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Argonne National Laboratory

APPLIED MATHEMATICS DIVISION SUMMARY REPORT

July 1, 1967 through June 30, 1968

ANL-7521
Mathematics
and Computers

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

APPLIED MATHEMATICS DIVISION
SUMMARY REPORT

July 1, 1967 through June 30, 1968

Wallace Givens, Division Director

Richard F. King, Assistant Director
for Publications and Reports

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PREFACE

The Applied Mathematics Division has two objectives:

1) to conduct research in applied mathematics, numerical analysis, theory and practice of computation, and design of computer and information processing equipment;

2) to provide mathematical, computer programming, and computational support for the research and development programs of the Laboratory.

Members of the Consultation and Research Section carry out their own independent research in various aspects of mathematics and programming. They are also available to assist laboratory personnel by mathematical consultation, in problem formulation, and in selection of appropriate mathematical and numerical techniques, and to carry out analysis of problems.

The functions of the Computer Engineering Section are (applied) computer engineering research, and the development and design of computers and information processing systems having special application to the nuclear sciences. Film scanning and measuring devices are a continuing interest. Experiment control based on data collection and (usually partial) analysis has been developed in concert with scientists of other divisions. The Division has a responsibility for assessment of digital computer equipment acquisition throughout the Laboratory for its feasibility and compatibility. The Engineering Section is an essential resource in fulfilling this responsibility. Appropriate members of the Section are prepared to assist in the formulation, programming, and running of problems for the Analog computer or in some cases to accept the problem and carry out these services. A limited hybrid computer capability also is maintained to the extent suitable equipment may be shared with other projects.

Software research encompasses numerical codes in machine language for basic system support, numerical analysis of fundamental algorithms for implementation of mathematical processes, conceptual studies in such areas as data structure, design of novel compilers, and theorem proving by computer.

The Digital Computing Center operates the central computing facility and provides systems programming support for it. Through its Systems Programming Section, the Center engages in advanced systems development aimed at the enhancement of the services of the computing facility and at advancement of computer systems technology. Members of the Computing Center's Applied Programming Section work with scientists from other divisions in formulating and defining problems for solution on digital computers. Applied programmers then carry out the necessary programming and documentation to achieve the ends specified in the program design.

APPLIED MATHEMATICS DIVISION
Organization Chart
July 1, 1967 through June 30, 1968

Director: W. Givens

Executive Assistant: D. A. Davis
Staff Assistant: R. E. King

Secretaries: M. Johnson, N. Baran(E), E. Fletcher, D. Haight, S. Mueller(T), G. Ramsey

Receptionist: L. Zimmerman(T), R. Munson(E)

Publications and Reports

Assistant Director: R. F. King
General Codes Distrib.: *W. J. Cody

Secretaries: M. Jedlicka, G. Krause

Argonne (Reactor) Code Center

Head: *M. Butler
N. Kazich(T)
Secretary: L. Ranzini
M. Legan

DIGITAL COMPUTING CENTER

Head: W. Cowell
Assistant Heads: J. Gabriel, B. Garbow, M. Storm
Secretary: K. Connell

DIGITAL OPERATIONS

Operations Manager: C. LeVee
Asst. Oper. Manager: W. Greenhow

Scheduling

E. Fearnow, *Leader*
S. Amsler
M. Csepregi(E)
M. Guzzy(E & T)
A. Johnson
N. Koca
D. Koenig(T)
S. Morris
C. Taylor(E & T)

Keypunching

A. Turk, *Leader*
C. Linchester
C. Misiurewicz
E. Overall
P. Zebrowski(E)

Central Machine Operations

J. Berkley
L. Douglas — *Shift Leaders*
T. Unger

J. Bartm(T)
A. Bate
R. Bene
R. Bils
A. Burg
C. Caru
J. Clapp
R. Clink
N. Colem
C. Conca
H. Cranf
D. Cybor
W. Dough
T. Dutto
M. Froeh
A. Goldst
W. Hilt(E
S. Hoston
D. Huber(
R. Jarka(
W. Jones(
C. Kilty
E. Kolsto(E)
M. Lawler
R. Mallette(E & T)
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M. Megson(T)
J. Midlock
M. Monczynski(E)
C. Ogletree(E)
R. Page(E & T)
R. Parran(E & T)
B. Reinke(T)
J. Reiter
R. Rempert
K. Rich
G. Schlesselman(E)
E. Singletary
J. Sullivan(E)
A. Vahcic

Remote Station Operations

J. Beck
H. Krejci
J. Nelson
L. Nelson

SYSTEMS PROGRAMMING

Leader: R. Logan
Clerical: J. Beumer

D. Brooks
D. Carson
R. Clark
K. Dritz
*W. Greenhow
D. Herman(E & T)
A. Hirsch
A. Joseph
R. Krupp
J. Ohde
A. Sandrin
*L. Shalla
C. Smith
D. Snider(E)
R. Tannura
R. VanBuskirk

APPLIED PROGRAMMING

Exec. Secretary - Assignment & Review Board: M. Prastein
Secretarial: *K. Connell
Production Services: S. Katilavas

Experimental Science

D. Woodward, *Leader*
J. Anderson
J. Gregory
J. Gvildys(T)
J. Herman
A. Strecok

Engineering & Applied Systems

*M. Storm, *Leader*
F. Clark(T)
H. Carlson
C. Harrison
N. Jesse(T)
R. Julke
R. Mueller(T)
P. Pennock(T)
J. Scherer
W. Snow
J. Wenger

Theoretical Physics & Chemistry

*D. Phillips, *Scientific Leader*
C. Chamot, *Group Manager*
N. K. Clark(T)
J. Cohen(T)
M. Gabriel
M. Kraimer(E)
M. Matthies
F. Taraba
S. Zawadzki

Reactor Theory & Development

*G. Leaf, *Scientific Leader*
P. Walker, *Acting Group Manager*
S. Sparck, *Group Manager*(T)
L. Bryant
S. Chaffin
B. Chandler
T. Daly(E)
G. Duffy(T)
H. Greenspan
D. Neal
G. Jensen(T)
L. Just
J. Kaganove
A. Kennedy
E. Kovalsky(E)
L. Meyer
A. Rago
D. Schoengold(E)
J. Stork(E)
T. Thompson(E)
J. Zapatka(T)

CONSULTATION AND RESEARCH

MATHEMATICAL ALGORITHMS

++J. Boyle
J. Butler
M. Butler
W. Cody
*W. Cowell
*W. Givens
*R. F. King
G. Leaf
J. Lyness
D. MacLaren
J. Reynolds
F. Stetter(T)
D. Taylor
L. Wos

MATHEMATICAL ANALYSIS

I. Abu-Shumays
E. Bareiss
P. Brockwell
R. Buchal
J. Cook
T. Hughes
J. Moyal
D. Phillips
V. Pless(T)
J. Pool
W. Smith(T)
J. VanRyzin(T)
*D. Woodward
++J. Zgrablich

PROGRAMMING DEVELOPMENT

Logical Methods

*L. Wos
L. Shalla

Numerical Methods

*W. Cody, *Leader*
N. A. Clark
K. Hillstrom
D. Jordan
V. Klema(E)
*J. Lyness
K. Paciorek
E. Thieleker

Partial Differential Equations

*T. Hughes
*D. Taylor
W. Wessel

ANALOG COMPUTING CENTER

F. Morehouse, *Leader*
A. Winiecki(T)

Technical Support:

F. Mal

COMPUTER ENGINEERING

D. Jacobson, *Head*
L. Amiot
R. Aschenbrenner(T)
D. Hodges
W. Lidinsky(E)
N. Natarajan(E)
F. Salter
C. Shelman
R. Vonderohe

Technical Support:

W. Ball(T)
R. Barr
J. Becker
R. English(E)
R. Foster
H. George
J. Haasl
B. Kroupa
F. Sato
R. Schwanke
N. Sobol
V. Tantillo
R. Wehman
G. Wittmus(T)

Drafting:

V. Grynczyk

(E) Entered during period.
(T) Terminated during period.
* Supplementary listing.
++ Special Arrangements:
J. Boyle - Dissertation appointment, Northwestern University.
J. Zgrablich - Resident Student Associate from Argentina.

ORGANIZATION CHART (Cont'd.)

TEMPORARY PROGRAM

SUMMER 1967	LONGER TERM	SUMMER 1968 (To June 30)
Resident Research Assoc.	Staff	Resident Research Assoc.
R. Blum	I. Abu-Shumays	R. Blum
W. Gautschi	J. Boyle	A. Ramsay
B. Levinger	F. Stetter	R. Sweet
	J. Zgrablich	C. Wilcox
Resident Student Assoc.		Resident Student Assoc.
M. Goldberg		G. Goldbogen
D. Johnson		J. Landwehr
D. Rocke		D. Rocke
Student Aides		Student Aides
A. Bradley		J. Dallman
R. Dreyer		D. Donohue
J. Glover		E. Giegler
L. Leibovich		W. Jung
J. Marentic		T. Mueller
D. Richards		C. Narz
E. Rozema		J. Patterson
		A. Ramp
		J. Urbaniak
		Temporary Clerks
		L. Gavin
		J. Manning

CONSULTANTS

R. A. Aschenbrenner, Electro Mechanical Research, Inc.
G. Birkhoff, Harvard University
R. Blum, The University of Chicago
W. W. Boone, University of Illinois
H. Cohn, University of Arizona
R. Courant, New York University
J. Douglas, Jr., University of Chicago
M. J. Flynn, Northwestern University
L. D. Fosdick, University of Illinois
C. W. Gear, University of Illinois
M. Golomb, Purdue University
A. A. Grau, Northwestern University
M. G. Keeney, Michigan State University
A. Lent, Northwestern University
W. F. Miller, Stanford University
J. H. Morrissey, Morrissey Associates Inc.
T. W. Mullikin, Purdue University
A. Newell, Carnegie-Mellon University
G. Robinson, Stanford University
J. A. Robinson, Rice University
N. R. Scott, University of Michigan
I. E. Segal, Massachusetts Inst. of Technology
A. H. Taub, University of California
H. C. Thacher, Jr., University of Notre Dame
R. J. Thomas, Depauw University
R. S. Varga, Case Western Reserve University
C. H. Wilcox, University of Arizona
A. Wouk, Northwestern University

COMPUTER SYSTEMS AND LANGUAGES

1. Installation of IBM System 360 Computer Complex

A. System Description

Installation of System 360 equipment in the Applied Mathematics Division began in June 1966 with a Model 50 and a complement of peripheral devices. In the fall of 1966, the magnetic core memory of the Model 50 was expanded, and then, beginning in June 1967, a Model 75 was added to give the configuration shown in the figure.

The more interesting features of the complex include the direct channel connection between the two main frames, the sharing of files (auxiliary storage devices) between the processors, and channel separation for accessing files of the same device type on the Model 75.

With the direct connection between the main frames, the Model 50 is used as support to the Model 75 in a sequential batch processing mode. The Model 50 handles all system input and output data, schedules the jobs, and controls and accounts for the use of the main processor. These tasks are accomplished by use of the IBM Attached Support Processor (ASP) system.

The sharing of files permits a more efficient use of the devices and offers an opportunity for the development of significant uses of the two computers in only faintly dependent modes. Since the sharing of one 2314 disk file provides an expansion of file capacity to the Model 75, systems residence and user scratch areas may be allocated over several volumes, and on different channels, while permitting a large number of private volumes either to be in operation or to be waiting in readiness for the parent job. Moreover, while large batch jobs are being processed in the main computer, the support computer may be servicing file management requests without the moving of volumes from one unit to another.

The relatively inexpensive addition of two channel-switch features and switching units increased the efficiency of operations on the 75 by permitting parallel access to different units of the same device type.

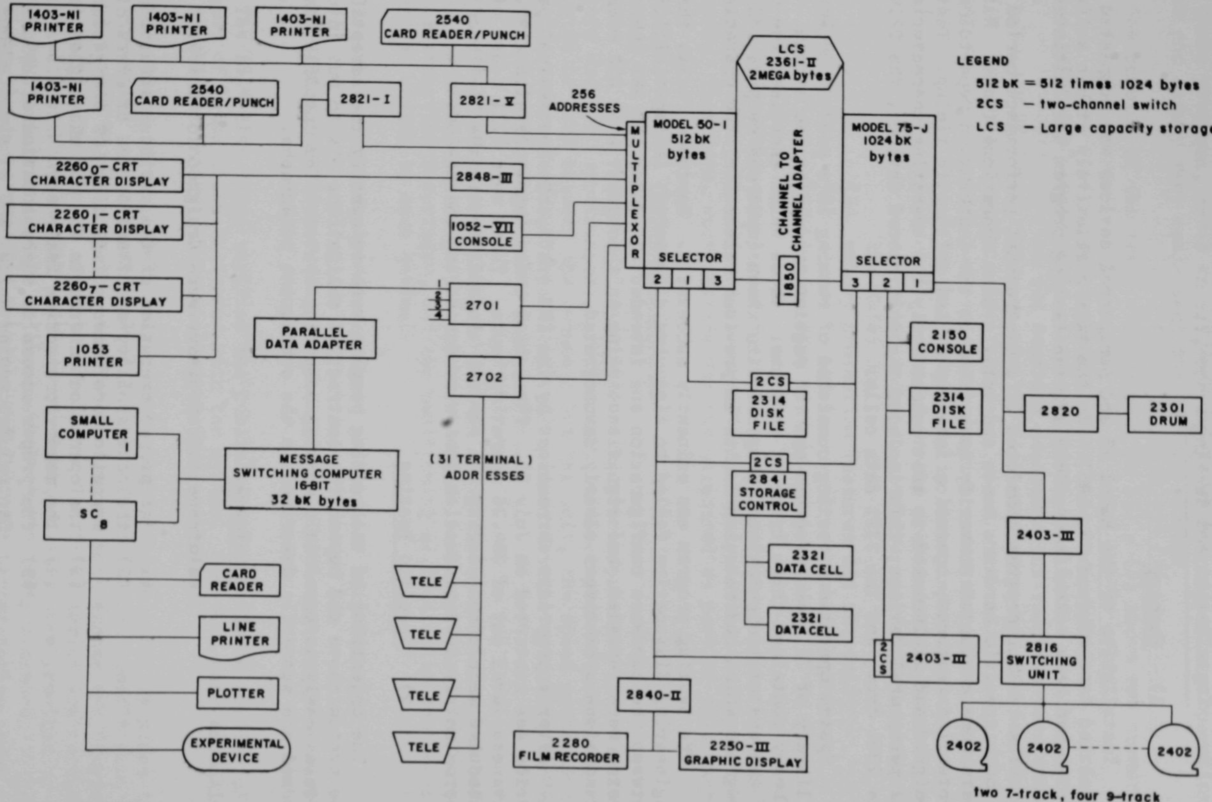
The initial allocation of system space to system processors was based on known and predicted characteristics of the Argonne job stream. The production system was designed to:

(a) minimize system interference (overhead) in job stream processing, and

(b) provide the user with as many of the resources and flexibility of the system as possible.

The system processors were made resident on three devices, the 2301 drum and two 2314 disk packs, according to frequency of usage; the unused space on each device was made available as user scratch areas. The resident modules of the 360 Operating System OS were selected to minimize direct access references while preserving a reasonable amount of free magnetic core memory. Procedures of job control language were designed to simplify the use of the system processors, and processor options were selected to provide the programmer with useful, but not extraneous, information.

ARGONNE NATIONAL LABORATORY
APPLIED MATHEMATICS DIVISION
S/360 CONFIGURATION



B. Installation and Testing

1) Summary

Installation of the Model 75 and peripheral devices was completed on the scheduled date of June 30, 1967. By the time a relatively stable software system had been established, July 17, the testing program was initiated.

The testing program consisted of a contractual performance period and of both specific hardware tests and total system operations tests. Mainframe tests were conducted to verify such items as the instruction repertoire, memory protection features, operation interrupts, and arithmetic timing. Tests were designed and implemented to test exhaustively the operating characteristics of all peripheral devices; this included the unit record devices, the 2314 disks, the 2301 drum, and the 2321 data cells.

System operations testing consisted of running in a production environment a library of 71 known programs and the regular production job stream. The library contained three types of programs: those which exercised the compilers of the system, computational programs with known input and output, and a set of programs which had revealed faults in previous releases of the operating system.

The testing program was eminently successful. Hardware faults that the engineering diagnostics failed to find were discovered, incompatibilities between the hardware configuration and intended use under the 360 Operating System were revealed, and significant gains in throughput with ASP over a stand-alone system were clearly demonstrated.

After appropriate corrections by the IBM staff, the contractual performance period was restarted on July 31. The period ended August 29 with a 97.7% effectiveness level out of 304.26 operating hours. There were 7.11 hours of unscheduled maintenance during the period. In addition to the 71 library programs, approximately 3000 production jobs were run during the period.

2) Specific Testing

The objectives of the testing program were to certify the acceptability of the system above and beyond the contractual obligations and to put into production as early as possible a working computing system. The specific tests performed are summarily described in the subsequent paragraphs.

(a) Mainframe.

Mainframe test programs were designed to verify:

(1) the proper execution of the entire instruction set;
(2) the accessibility and flawlessness of every bit of magnetic core memory, including LCS (Large Core Storage);
(3) the operation interrupts for all unassigned order codes;
(4) the memory protection features;
(5) the proper access to every location of LCS from both Central Processing Units (CPU's) simultaneously; and
(6) the quoted arithmetic speeds.

These programs, three in all, operate independently of any operating system and occupy very small sections of core storage.

The results of the tests with respect to (1) - (6) above are summarized:

(1) the instruction set executed properly;
(2) no problems were discovered in the main core, but on two separate occasions LCS failures were established; the IBM diagnostic programs did not reveal the LCS failures;
(3) some illegal operation codes cause interrupts only if their execution is attempted under control of OS, or if attempted in the problem state; some illegal operation codes do not give operation interrupts on the Model 50;
(4) memory protection features did not fail;
(5) access to LCS was proper from both machines;
(6) instruction timings were verified.

The arithmetic accuracy of the system requires more lengthy testing than the test schedule allowed, and is significant mainly in relation to arithmetic routines. Therefore, such testing was not attempted as part of this exercise.

(b) Peripheral devices

For the unit record equipment (2540 card reader/puncher, 1403-N1 line printers and 1052 typewriters), procedures were developed for measuring transfer rates of data between the channels and the unit, the speed performance of the unit, the performance capabilities of several devices operating concurrently, and special features unique to each device.

For the direct access storage devices (2314 disks, 2301 drum and 2321 data cells), programs were devised to check the oxide surfaces, the input/output (I/O) instruction repertoire, and the positioning of read/write and accessing mechanisms unique to each device.

The unit record equipment was found to be quite satisfactory.

No drum errors occurred although many runs of the test programs were made.

The 2314 disk tests verified the published speeds and the quality of the surfaces of those disks delivered with the system. However, many anomalies were discovered in IBM's surface analysis program, DASDI.

The 2321 data cells were tested particularly for reliability since they are a novel and very complex type of device. The principal benefit from the cell tests was to point up the need for continuing maintenance and "tuning" on the cells. Two series of tests were run. The first series was conducted on the cells without special preparation, i.e., as they were provided by IBM under normal maintenance. In this series of 28,000 strip accesses, 72 permanent errors occurred and 201 corrected errors. The second series began with new strips of tape. The error rate continued very high for the first 2,000 accesses. After very careful maintenance, only one permanent error and ten corrected errors occurred in 32,000 accesses.

(c) System Operation.

Hardware operability is a necessary condition to system acceptability, but it is not sufficient; the system as a hardware-software package must do the work of the Laboratory within acceptable levels of reliability and confidence. System operation was evaluated with a developed library of production and production-like programs and with careful statistical observation of real production during the performance period.

The test library consisted of 71 programs organized into three groups: (1) processor (compiler, etc.) testing and evaluation; (2) executable programs with data; and (3) programs which demonstrated errors in the operating system noted prior to the installation of June 1967. Most of these programs had been run on the Model 50 during fiscal year 1967; some were specially constructed to test newly delivered system processors. Every processor in the operating system was checked.

During the initial performance period beginning July 17, numerous hardware and software faults were discovered through the use of the test library. Most of these were corrected through engineering changes to the hardware and special modification to the Operating System. The job stream timing tests showed an improvement ratio of from 7:1 to 10:1 for the 50/75 system over the stand-alone 50 system. Compiler performance improvement ratio varied from 5.5:1 for Fortran G to 15:1 for Fortran H. The magnitude of the Fortran H improvement is due in large measure to the use of the 2301 drum for system processors.

2. IBM System/360 Development

A. Film Plotting

A subroutine package containing 39 subroutines for using the IBM-2280 Film Recorder was developed during fiscal year 1968. The subroutines may be invoked by using the CALL statements of either the FORTRAN or PL/1 programming languages. These subroutines form a hierarchy of capability from a single, general-purpose plotting routine to a calling capability for the assembly language graphic macro instructions. Characters, points, and vectors may be plotted, and the buffer of the 2280 controller may be managed directly through these routines. The package gives the FORTRAN and PL/1 programmer essentially all the flexibility available to the assembly (machine) language programmer, but simplifies the use of the film recorder.

B. Large Core Storage (LCS)

This large memory unit, with an access time of 8 microseconds, is physically attached to the upper end of an S/360's main faster core storage. Its speed is less than the data transfer rate of the 2301 drum. The S/360 Operating System does not make any distinction between LCS and the main magnetic core memory. Therefore, with a 2301 drum attached, it is impossible to use LCS without (1) modifying the operating system and (2) providing dynamic control over its use to the programmer. Without a 2301 drum, LCS could have been used without distinguishing it from fast core; the overhead penalties, however, are prohibitive.

In the fall of 1968, the LCS development program was completed. The program consisted of modifying the Operating System to provide the following specific capabilities:

1) specify at start-up time the amount of core available to the system and permit start-up without any special LCS switch setting;
2) FORTRAN and PL/1 program dynamic management of all magnetic core, including LCS;
3) automatic release and dump of only the used portion of core storage at job or job step termination.

Checkout of the complete system began in the summer of 1968.

C. System Performance and Computer Utilization.

In the Applied Mathematics Division Summary Report for fiscal year 1967, ANL-7418, an approach to the quantitative measurement of the efficiency of the System/360 with respect to the Argonne job stream was described. Phase 1 of a 3-phase project has been completed, and work is continuing toward the other phases. Phase 1 consisted of the development of a monitoring system for the Attached Support Processor (ASP) system and the development of a basic set of programs for analyzing the data collected with the monitor. Phase 2 of the program is the development of a monitoring program for the operating system, OS/360. Design data and parameter selection criteria are being analyzed and evaluated. The monitor will be designed for and implemented in the MVT (Multiprogramming with a Variable Number of Tasks) version of OS. Phase 3 of the program consists of extensive data collection and analysis.

Phase 1 of the Dynamic Status Recorder (DSR) system has been implemented to serve as a tool for gathering data about the operation of a computing system. It is imbedded in the software monitor that controls the scheduling and peripheral input-output functions of the system. The output of DSR is a magnetic tape which contains elements representing the various events that have occurred. This tape allows simulation of the operation of the monitor so that another program may analyze the functions of the system in detail at a more leisurely pace.

Such a simulator has been written. It is structured so that each event that may occur is processed by a separate subroutine. In addition, a user's routine may also be executed for those events that describe the operation of a particular subsystem of the support processor monitor. The group of user's routines may tally events or produce averages, standard deviations, and other statistical measures of activity; these are formatted and printed at the end of the analysis.

Several analyses have been performed on some limited samples of data. The results have verified theoretical studies of the ASP system within reasonable expectations and have provided extensive data in other areas of ASP performance. These studies and data collection are continuing.

Although the dynamic status recorder was designed for a particular type of operating system for the solution of practical systems problems, it nevertheless is of some theoretical interest. It provides a means for quantitatively evaluating various algorithmic approaches for handling necessary computing functions, i.e., those common to any computing system, with given classes of equipment.

The method of DSR, though implemented in ASP, is generally applicable and usable for the collection of quantitative data on parameters which are system independent. Though the cost of implementing the method is high, the overhead of the system during operation is negligible.

3. Computer Production System Support

Production system support for the major computers of the Applied Mathematics Division's Digital Computing Center consists of:

(a) designing and building the operating system from the modules supplied by the manufacturer;
(b) modifying the system to suit the Laboratory needs;
(c) diagnosing and correcting (both where possible) system operation problems;
(d) developing system statistics on performance and job stream characteristics;
(e) providing user and operator consultation, reference, and educational services.

The present system design utilizes the link between the IBM 360 Model 50 and the Model 75 for sequential job processing on the Model 75. The Model 50 ASP (Attached Support Processor) system handles the activities for preparing — job input and device allocation — and finishing — job output and device allocation — a job, and schedules the jobs for the Model 75. The operating system in the Model 75 is structured to process jobs in a sequential schedule. Development work for restructuring the Model 75 operating system and ASP to permit the concurrent processing of as many jobs as the core size allows in the Model 75 is commencing.

The Model 50 operating system is structured to permit the concurrent running of other systems and jobs with ASP in a memory partition of lower execution priority than ASP. This lower priority partition is used to run Type 2250 interactive graphic display jobs, the Argonne conversational system "RESCUE," and other system development jobs on a scheduled basis. If the multijob processor for the Model 75 and ASP is successful, the 2250 jobs can be run without economic penalties on the Model 75, and RESCUE may occupy the partition for longer periods during the day.

Ten major operating systems have been installed since delivery of the IBM 360 Model 75 on June 30, 1967. In addition, over 250 updates and corrections have been made. Major Argonne modifications to the 360 Operating System (OS) and ASP have been made to enhance the capabilities of the system for Argonne computing needs. The two most significant modifications to OS are (1) the addition of a set of system resident routines and (2) the modifications of OS modules and addition of new modules for programmer-controlled use of the Large Core Storage (LCS). A byproduct of the LCS support is a generalized capability in FORTRAN programming to manage magnetic core storage dynamically in a manner similar to what exists in PL/1. The set of system-resident routines includes much of the Applied Mathematics Division mathematical subroutine library, the LCS routines, a hierarchy of film-plotting routines for the 2280 film recorder, and CALCOMP (mechanical) plotting routines.

The major modifications to ASP include:

(a) operator console support for the IBM 2741 typewriter and Teletype Model 33;
(b) accounting routines for handling account charges automatically;
(c) a job stream priority scheduler;
(d) support for 2321 Data Cells as setup devices (later obsoleted by full OS support);
(e) drivers for the 2280 Film Recorder;
(f) the Dynamic Status Recorder;
(g) a generalized tape-to-printer program for printing any seven- or nine-track tape of unknown characteristics.

In addition, there were numerous modifications which, though minor to effect, made significant improvements in the operation of the system.

4. RESCUE, A Responsive Computer User Environment

"RESCUE" is the mnemonic used to refer to the Argonne system for conversational computing on the IBM SYSTEM/360 Model 50. The purpose of the system is (a) to improve batch processing (sequential) capabilities by making easier many of the standard computer uses which are awkward and time inefficient in the batch mode, e.g., syntax error analysis and information management, and (b) to provide avenues for computer usage which are not available through the Operating System, e.g., discipline-oriented languages and user-defined interactive processors.

In the previous summary report, five categories of user facilities were described as preliminary objectives of the development project: information management, preprocessing of major programming language texts, remote job entry, interpretive computing, and ephemeral computing.

The RESCUE system is made up of three major software components: (1) the RESCUE Control Program (RCP), (2) the RESCUE Subsystems (resource systems, such as DISCOM and PL/1), and (3) the interface between RCP and the subsystems. The Control Program, designed for interactive computer usage only and for study of such usage, is modular in form and intended to be easy to maintain through on-line debugging of RESCUE modules. It incorporates functional components needed by all subsystems, controls data areas and time slices, and loads and controls execution modules. It also handles input/output, management of storage requirements, console attention requests, and linkage among the program modules (Processors) of which each RESCUE subsystem is composed.

The initial user facilities are those which are basic to the further development of user facilities and those which are most appropriate for supplementing and improving batch processing. These are:

(a) Interpretive Computing.

A strictly mathematical language, DISCOM, has been developed for the unsophisticated computer user. It is an experimental interpretive system; this means that execution is performed on a statement-by-statement basis. It contains arithmetic and relational operators, array specifications, input/output statements, transfer control statements, repetitive execution controls, and a library of mathematical functions. In addition a user may change (edit) his algorithm, try sections of it, or interrupt execution. Current specifications call for elementary matrix operations.

(b) On-line Data Storage and Editing Facilities.

The file management system provides a versatile method of storing collections of data on secondary direct access and sequential devices, with the ability to access or rewrite any record in the file and to protect the file from unintentional errors and unauthorized tampering. The file management system views users in a generalized sense to include system processors. Thus file maintenance capabilities exist for the control program, DISCOM, and any other system processor as well as for terminal users. Finally, the system data interfaces with the batch operating system, OS, so that OS and RESCUE files may each be made available to the other system. Design effort is directed toward achieving initially the following general facilities:

(1) LIST the content of the file directory or specified information pertaining to a selected file;
(2) PRINT the entire or selected portions of a file;
(3) DELETE a file or set of files;
(4) CHANGE the name or mode of a file;
(5) COPY an existing file;
(6) EDIT the content of a file;
(7) BUILD either an OS/360 file from a RESCUE file or conversely.

(c) PL/1 Language Processing.

The PL/1 language processing system consists of a text builder, a syntax analyzer, and a diagnostic controller. The purpose of the system is to provide the user with a facility for on-line building and correction of PL/1 program files. Syntax errors are announced to the user as each statement is completed. He may make corrections before entering other statements or at a later time.

It is expected that the main use of the system will be as a generator of small, partly error-free PL/1 programs to be converted into OS files and submitted to the batch system for compilation and execution. Preprocessing provides an increase in the probability that the batch job will actually get to the execution phase. Thus, by spending a small amount of time at a console, a user may save hours of batch turn-around time that would have turned up errors severe enough to prevent execution.

(d) FORTRAN IV Language Processing.

Essentially the same facilities as described for PL/1 are under study.

(e) Remote Job Processing.

Remote job processing consists of those activities required to submit a job to the OS batch system, inquire of the status, and receive its output. To achieve these facilities for a user at a console, RESCUE is interfaced with the Attached Support Processor for the SYSTEM/360(ASP) to look like an input reader, an output writer, and a console operator. The console user, however, merely instructs RESCUE to submit his program and data to ASP to inquire of its state in the batch system, or to retrieve the batch output either for browsing on a cathode ray tube display or for printing.

In addition to the user facilities, supervisory processors have been developed to aid in the on-line development of the system. These currently include:

(a) The PAL system, a debugging and checkout tool used to test the page management, attention handling, and linkage management machinery of the RESCUE control program.

(b) The RESCUE Test System (RTS), a single Processor system with which the RESCUE programmer can test various RESCUE control program functions while on-line at a RESCUE terminal. The programmer can, for example, cause various program faults (to check out the error handling machinery), cause the system to become computer bound (for the purpose of measuring the system's time slice quantum), and so forth.

(c) TELTEST1, a processor written to debug the terminal-dependent input/output modules. The processor checks the general flow of terminal I/O and those terminal features unique to the RESCUE system.

(d) SYSDMP, a processor written to aid in debugging RESCUE systems. The processor will display contents of system tables and control blocks, and any part of the core storage. Table and control block format displays the symbolic name of the table element followed by its contents.

5. Transformational Grammar and Programming Languages

Recent interest in methods for defining computer programming languages has centered on the problem of specifying the semantics, or meaning, of these languages. One approach to this problem is to define the meanings of the complex statements of a programming language in terms of groups of equivalent simple statements whose meaning can be presumed known.

The grammatical transformations introduced by Chomsky to describe the transformation of an active sentence in English into its passive counterpart have been adapted for use with programming languages and used to express such definitions. A transformational description of a method for improving the efficiency of loop statements in Algol 60 has been developed, and transformations are being applied to the description of identifier denotation, which is the process of associating the identifiers in an Algol 60 program with their declarations. (This latter application is an extension of earlier work on algorithms for identifier denotation which is currently being revised for publication.) Also being sought are theorems giving criteria for the termination of the algorithm performing the transformations.

6. Integrated Macro Processing

In relation to a programming language, the term "macro processing" may be taken to mean compile*-time processing controlled by definitions expressed in the language. A facility for this sort of processing is standard in most machine assembly language systems; but the form of macro processing in these systems is

*Compilation is the process of generating computer machine-language instructions from source statements written in some programming language; usually each statement results in several or many machine instructions. Each assembly language statement, on the other hand, normally leads to just one machine instruction.

not well suited for use with higher level procedural languages such as Algol or PL/1. The principal problem is that assembly language macro processing is carried out as a separate operation before the basic assembly process, while in higher level languages it is both necessary and desirable to integrate macro processing with other parts of the compilation process.

In an approach recently developed, macro processing takes place after syntactic analysis of the source program and along with the processing of declarations. The advantage of this is twofold. First, in writing macro definitions, the programmer is freed from concern with the details of syntactic analysis; instead of working with strings of characters, he works directly with entities that seem natural for programming, e.g., integers, identifiers, and expressions. Second, when a macro procedure is executed at compile time, it may access information contained in declarations already processed. A facility for this sort of macro processing will be a major part of the general-purpose Extendible Programming System (EPS).

7. General-purpose Programming Languages

Probably the most important current goal in the design of general-purpose programming languages is to achieve simplicity without sacrificing generality. In an attempt to meet this goal, a simple but surprisingly general language called "Gedanken" has been defined. Its name implies an analogy with gedanken-experiments in physics, i.e., it is intended to be an idealized model of certain important aspects of programming languages, rather than a practical language itself.

The design of Gedanken is based on two principles:

(1) The formalization of addressing or "naming" used in Algol 68, which makes a precise distinction between a value and an object which takes on values.

(2) Any value which is permitted in some context in the language must be permitted in any other meaningful context. Thus, for example, procedures and labels, which are allowed to be input arguments to procedures, are also allowed to be results of functions or values of variables.

These principles have the following consequences:

(1) A compound data structure such as an array is a special case of a function (mapping the subscripts of the array into its elements). This allows any such structure to be replaced by a functional procedure which computes the elements of the structure as they are accessed.

(2) Unorthodox control processes such as co-routines and quasi-parallel processes (e.g., in discrete simulation languages) can be realized by using label variables.

(3) The stack discipline of program variables and control information, which characterizes conventional programming languages, breaks down and must be replaced by a dynamic storage allocation mechanism.

The preparation of special function routines has paralleled that of approximation work for the exponential integrals E_1 and Ei and for the negative exponential function. Work on some double-precision routines for the 360 will recommence when floating point engineering changes scheduled for October 1968 have been completed. It is anticipated that a number of routines will be needed to replace some of the double-precision routines in the IBM FORTRAN IV library. Another addition to the library is a KWIC SØRT program.

Work in progress includes a subroutine for the evaluation of Fourier coefficients, routines for the complex gamma function, the zeta function, and the complex error function, and preliminary work on a program to aid conversion of CONTROL DATA 3600 FORTRAN programs to IBM S/360 FORTRAN IV. Planned work involves polynomial root finders and a variety of curve-fitting programs (discrete linear Chebyshev fits, spline fits, etc.)

11. New Library Routines

ANL B252S	ARGSINH	W. J. Cody	360 routine to evaluate the hyperbolic sine or cosine of a single-precision floating-point variable.
ANL B354S	DEXP	N. W. Clark	360 routine to compute the double-precision exponential of a double-precision floating-point number.
ANL B456S	DCUBRT	K. Paciorek	360 routine to compute the double-precision cube root of a normalized double-precision floating-point argument.
ANL B457S	ARGPOWER	D. Jordan	360 routine to evaluate A to the power B for single-precision floating-point arguments A and B.
ANL B458S	ANLDPOWR	D. Jordan	360 routine to evaluate A to the power B for double-precision floating-point arguments A and B.
ANL C250S	CUBIC	B. Garbow	360 FORTRAN routine to find the three roots of a cubic polynomial equation.
ANL C251S	QUARTI	B. Garbow	360 FORTRAN routine to find the four roots of a quartic polynomial equation.
ANL C252S	RSSR	B. Garbow	360 FORTRAN subroutines (10) to find the zeros of a polynomial with real coefficients.
ANL C353S		D. Jordan	360 routine to evaluate certain angular momentum coefficients.

The main goal of future research is to develop constructs such as type and scope declarations which can be added to Gedanken to permit efficient implementation and error detection without restricting generality.

8. Programming Language for Least Squares Fits

When a scientist has a set of data to which he would like to fit an appropriate function, he often discovers that his first attempt could probably be improved by adding more terms or even changing the function's form. This means that the computer program solving such a least squares fitting problem must each time be laboriously rewritten — either by the scientist himself or by a computer programmer. The task is complex, tedious, and slow.

To help alleviate the difficulty, a special-purpose language and a corresponding IBM 360 computer program to translate this language have been developed. The result is that a minimal description of the particular function desired suffices to determine a best fit. The process may then be readily repeated with other candidates for an improved fit.

The entire processing program accepts function and partial derivative information, plus the observed data, generates a FORTRAN code for the suggested fit, and proceeds to compile and execute this code. There is also provision for a sophisticated user to add FORTRAN statements of his own. Davidon's minimization procedure is used in the fitting, and the translator itself is written for convenience in the PL/1 language; for the user, however, these are unimportant details.

Extensions to provide graphs and auxiliary calculations are now being examined.

9. Subroutine Certification

Both a philosophy towards certification of numerical subroutines and the particular techniques used at Argonne in certifying function subroutines have been explained in papers just completed. These ideas have been used in certifications of five routines from the IBM Scientific Subroutine Package as a contribution to the SHARE Numerical Analysis project. The reports are to appear in the Share Secretary Distributions.

It is planned to repeat certification of the IBM FORTRAN IV library on the modified IBM library. Work should begin on this project as soon as certain floating point engineering changes have been completed.

The performance of five adaptive quadrature schemes applied to definite integrals with peaked integrands has been measured. A report intended for the open literature is in preparation.

10. Computer Subroutine Libraries

Some fifty-four routines have been added to the computer subroutine libraries, most of them for the IBM System/360 but several for the still-active CONTROL DATA 3600. Major contributions have been made in the area of special functions of mathematical physics and in that of matrix calculations, where a whole set of J. H. Wilkinson's codes have been translated with his cooperation into the FORTRAN IV language for the IBM S/360.

ANL C354S ELLIPK K. Paciorek

This 360 routine evaluates the complete elliptic integral

$$K(k^2) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - k^2 \sin^2 \phi}}$$

given k^2, a single-precision floating-point number.

ANL C355S ELLIPE K. Paciorek

This 360 routine evaluates the complete elliptic integral

$$E(k^2) = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2 \phi}\, d\phi$$

given k^2, a single-precision floating-point number.

ANL C367S GAMMA/ ALGAMA K. Hillstrom

360 routine to evaluate the gamma function or the natural log of the gamma function of a real, single-precision, floating-point argument x.

ANL C368 EONE D. Jordan

3600 routine to compute the exponential integral

$$E_1(x) = -Ei(-x)$$

$$= \int_x^{\infty} \frac{e^{-t}}{t}\, dt \quad \text{for } x > 0$$

ANL C368S EONE D. Jordan

360 routine to compute the exponential integral as stated above in ANL C368.

ANL C369S DEONE D. Jordan

360 routine to compute the exponential integral

$$E_1(x) = -Ei(-x)$$

$$= \int_0^{\infty} \frac{e^{-t}}{t}\, dt$$

in double precision.

ANL C370S BESJY D. Jordan

360 routine to compute a double-precision sequence of Bessel functions either of the first or second kind; i.e., either

$$\{J_v(x), J_{v+1}(x), J_{v+2}(x), \ldots, J_{v+N}(x)\}$$

or $\{Y_v(x), Y_{v+1}(x), Y_{v+2}(x), \ldots, Y_{v+N}(x)\}$

for given values of v, x, and N.

ANL C371S BESIK D. Jordan

360 routine to compute a double-precision sequence of exponentially scaled modified Bessel functions; either

$$\{e^{-x}I_\delta(x), e^{-x}I_{\delta+1}(x), e^{-x}I_{\delta+2}(x), \ldots, e^{-x}I_{\delta+N}(x)\}$$

$$\text{or } \{e^{x}K_\delta(x), e^{x}K_{\delta+1}(x), e^{x}K_{\delta+2}(x), \ldots, e^{x}K_{\delta+N}(x)\}$$

for given values of δ, N, and x.

ANL C372 CHIPRB K. Paciorek

This 3600 function subprogram calculates

$$\frac{1}{2^{n/2}\,\Gamma(n/2)} \int_x^\infty z^{n/2-1}\, e^{-z/2}\, dz \qquad (x \geq 0,\ \ n \geq 1),$$

which represents the probability that χ^2 for n degrees of freedom exceeds x.

ANL C372S CHIPRB K. Paciorek

This 360 double-precision function routine calculates same as above in ANL C372.

ANL C373S DELIPK K. Paciorek

360 double-precision function subprogram evaluates the complete elliptic integral

$$K(k^2) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - k^2 \sin^2 \phi}}$$

given k^2, a double-precision floating-point number such that $0 \leq k^2 < 1$.

ANL C374S DELIPE K. Paciorek

360 double-precision function subprogram to evaluate the complete elliptic integral

$$E(k^2) = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2\phi}\; d\phi$$

given k^2, a double-precision floating-point number such that $0 \leq k^2 \leq 1$.

ANL C376	**EXPINT**	K. Paciorek	This 3600 single-precision function subprogram calculates $$Ei(x) = \int_{-\infty}^{x} \frac{e^t}{t}\,dt, \quad \text{for } x > 0$$ $$Ei(x) = -E_1(-x) = -\int_{-x}^{\infty} \frac{e^{-t}}{t}\,dt, \quad \text{for } x < 0$$ $$E_1(x) = \int_{x}^{\infty} \frac{e^{-t}}{t}\,dt, \quad \text{for } x > 0$$ and $e^{-x}Ei(x)$ for all x.
ANL D154S	**CMQUAD**	K. Hillstrom	360 routine for modified Chebyshev quadrature to evaluate the definite integral $\int_a^b f(x)dx$ of a function (integrand) of a real double-precision floating-point argument x over the interval $a \le x \le b$.
ANL D155S	**SIMP**	K. Hillstrom	360 routine for adaptive Simpson rule quadrature to evaluate the integral $\int_a^b f(x)dx$ of a function (integrand) of a real double-precision floating-point argument x over the interval $a \le x \le b$.
ANL D156	**EXTRAP**	K. Hillstrom	3600 routine to evaluate the definite integral $\int_a^b f(x)dx$ of a function (integrand) of a real single-precision floating-point argument x over the interval $a \le x \le b$.
ANL D157S	**ASIMP**	K. Hillstrom	360 routine for adaptive Simpson rule quadrature to evaluate the definite integral $\int_a^b f(x)dx$ of a function (integrand) of a real double-precision floating-point argument x over the interval $a \le x \le b$.
ANL D158S	**ANC4**	K. Hillstrom	360 routine for adaptive quadrature, using the five-point Newton-Cotes formula, to evaluate the definite integral $\int_a^b f(x)dx$ of a function (integrand) of a real double-precision floating-point argument x over the interval $a \le x \le b$.

ANL D254S	DEGEAR	C. W. Gear and N. W. Clark	360 program for the numerical integration of ordinary differential equations with initial value boundary conditions. This program numerically integrates the set of n equations, $$y_i^{(p_i)} = f_i\left(x, y_1, y_1', \ldots, y_1^{(p_1-1)}, y_2, y_2', \ldots, y_n^{(p_n-1)}\right) \quad i=1,2,\ldots,n$$ where $$y^{(p)} = \frac{d^p y}{dx^p} .$$
ANL D255	DFBND-DIFI	K. Paciorek	3600 double-precision routines which estimate the error in the Bulirsch-Stoer method for solution of a system of first-order ordinary differential equations.
ANL D255S	DFBND-DIFI	K. Paciorek	360 double-precision routines which estimate the error in the Bulirsch-Stoer method for solution of a system of first-order ordinary differential equations.
ANL D256	DFBDRV	K. Paciorek	3600 double-precision routine which provides input/output and control for use with the double-precision routines ANL D255 DFBND-DIFI to integrate a system of first-order ordinary differential equations.
ANL D256S	DFBDRV	K. Paciorek	360 double-precision routine which provides input/output and control for use with the double-precision routines ANL D255S DFBND-DIFI to integrate a system of first-order ordinary differential equations.
ANL E206S	LSQPOL	K. Paciorek	Given a set of N values of an independent variable X, with associated weights W, and one or more sets of corresponding values of Y; this 360 FORTRAN routine determines the coefficients of the polynomial(s) of degree M-1 which give(s) the best fit in the least squares sense to the set(s) of Y. In addition, the residuals, the weighted sum(s) of squares of residuals, and the error matrix are computed. The program is in double precision but changes for single precision as indicated on COMMENT cards in the statement listing.

ANL E209S	CALLSQ	K. Paciorek	This 360 routine provides the input/output and control needed to fit, in a least squares sense, polynomials of varying degrees to a set of observed values - using ANL E206S - LSQPOL.
ANL F105S	MATEQ, UNIQUE	B. Garbow	These 360 FORTRAN subroutines (2) solve the matrix equation AX=B and obtain the generalized inverse of A, where A is any rectangular NR x NC non-zero coefficient matrix and B is a matrix of constant vectors. In the case where this equation is unsolvable, a best solution in the least squares sense is obtained.
ANL F150S	HERM	V. Klema	Package of 360 routines to perform the Householder reduction and calculate the eigensystem of hermitian matrices.
ANL F154S	DOTP	D. Jordan	360 routine to get an accurate inner product of two vectors. This is done through multiple precision accumulation of the terms, thus eliminating the subtraction errors that are likely to occur when the precision of the accumulation step is no better than that of the individual vector components.
ANL F155S	HESSEN	V. Klema	360 routine to reduce a single-precision complex non-Hermitian matrix to upper Hessenberg form with a real lower subdiagonal.
ANL F156S	RAYCOR	V. Klema	360 routine to form Rayleigh corrections to eigenvalues of a real symmetric matrix. Real input parameters and results are double precision.
ANL F202S	EIGEN	B. Garbow	360 routine to find all scalar solutions, λ_i (including proper multiplicity), and the associated orthonormal vectors, x_i, to the matrix equation $Ax=\lambda x$, where A is a real, symmetric matrix.
ANL F250S	FRANCI	B. Garbow	360 FORTRAN package of three subroutines to find all scalar solutions, λ_i (including proper multiplicity), to the matrix equation $Ax=\lambda x$, where A is an arbitrary real square matrix.

ANL F251S	FRANCC	B. Garbow	360 FORTRAN package of three subroutines to find all scalar solutions λ_i (including proper multiplicity) to the matrix equation $Ax=\lambda x$, where A is an arbitrary complex square matrix.
ANL F252S	GEIGEN	B. Garbow	360 routine to find all scalar solutions, λ_i (including proper multiplicity), and the associated unit vectors, x_i, to the matrix equation $Gx=\lambda Fx$, where G and F are real, symmetric matrices with F positive definite.
ANL F255S	SDIAG	V. Klema	360 routine to find all of the eigenvalues and eigenvectors of a real symmetric double-precision matrix.
ANL F257S	TSTMTZ	B. Garbow	360 routine to generate a real symmetric matrix from a specified diagonal matrix. The eigenvalues, eigenvectors, with Euclidean norm 1, and the determinant of this matrix are also generated. This routine can be used to generate a pair of matrices which are inverses of each other.
ANL F258S	LRCHZ	V. Klema	360 routine which uses the LR algorithm, in double-precision arithmetic, to find the eigenvalues of a real symmetric matrix. Subroutines DECMPZ, for Cholesky decomposition, and RECMBZ, for multiplication of triangular matrices, are included in this package.
ANL F402S	MATINV	B. Garbow	360 routine to solve the matrix equation $AX=B$, where A is a square coefficient matrix and B is a matrix of constant vectors. The determinant and inverse of A are also obtained; indeed, inversion may be the sole aim in a particular usage.
ANL F453S	MATINC	B. Garbow	360 routine to solve the complex matrix equation $AX=B$, where A is a square coefficient matrix and B is a matrix of constant vectors. The determinant and inverse of A are also obtained; indeed, inversion may be the sole aim in a particular usage.
ANL F454S	CROUT	B. Garbow	360 routine to solve the matrix equation $AX=B$, where A is a square coefficient matrix and B is a matrix of constant vectors. The determinant of A is also obtained.

ANL F455S	CROUTC	B. Garbow	360 routine to solve the matrix equation AX=B, where A is a complex square coefficient matrix and B is a matrix of constant vectors. The determinant of A is also obtained.
ANL G552S	RANF	N. W. Clark	360 FORTRAN routine to produce a uniformly distributed sequence of random numbers.
ANL K250S	Core to core conversion	D. Carson	This 360 routine will allow core to core conversion guided by a FORMAT-type specification. Conversion is either from internal machine representation to EBCDIC or vice versa.
ANL M151S	ANLKWIC	D. Jordan	The purpose of the 360 routine ANLKWIC is to provide Key-Word-in-Context (KWIC) listings from sets of discrete data items, an item consisting of up to 112 characters of text plus an 8-character retrieval code.
ANL Q054S	DATE	C. Smith and W. Cody	360 routine to obtain the current date in the Gregorian calendar, i.e., the current date in the form MM/DD/YY when MM is the month, DD the day of the month, and YY the year.

12. Abstracts of Computing Center Newsletters

The aim of the NEWSLETTER is to carry current information of interest to users of AMD computer services both for the IBM 360 Systems and for the CONTROL DATA 3600, plus related areas.

DIGITAL COMPUTING CENTER NEWSLETTER NO. 4 November 1967

- S/360 System News
  - ASP Control Cards and Programming Considerations
  - 360 FORTRAN IV In-Line Functions
  - Calcomp Plotting under ASP
  - 360 Applications Program Job Library
  - OS/360 Utility Program Notes
  - System Cataloged Procedures
- CDC-3600 System NEWS
  - Updated SCOPE System, SYS 10-17B
  - Disk File Control System Troubles with Overlays
- Miscellaneous Notes
  - Zero Priority Jobs on System/360 and Rate Changes
  - Computer Time Refunds
  - Systems Programming Consultation Changes
  - Magnetic Tape Storage
  - AMD Program Library Notes
  - Computer Users Fringe Benefits Revealed
  - Scrap Paper Explosion

DIGITAL COMPUTING CENTER NEWSLETTER NO. 5 April 1968

- S/360 System News
  - Updated OS/360 System, OS75 - 13.0
  - ASP System
  - Flowcharting on the S/360
  - Debugging Using an Object Module Library
  - User Contributions - Experience Talking
  - Modifications to the FORTRAN Subroutine Library
  - System Configuration
  - 2250 Interactive Graphics Availability
  - Data Cell (2321) Note
- 3600 System News (no entry)
- Miscellaneous Notes
  - Library Notes
  - Newsletter Distribution

DIGITAL COMPUTING CENTER NEWSLETTER NO. 6 June 1968

- S/360 System News
  - Updated OS/360 System, OS 75 - 14.0
  - ASP System - Job Priority Change
  - SYS1.AMDLIB - AMD Supplied Subroutines
  - Peripheral Computer Operations Requests for S/360
  - User Contributions - Experience Talking
  - FORTRAN IV Support for IFPEC
  - 2321 Data Cell Availability
  - FORTRAN IV In-Line Functions
- 3600 System News
  - Updated 3600 SCOPE System, SCOPE 10-17C
- Miscellany
  - Library Notes
  - New S/360 Package Available for Ordinary Differential Equations

NUMERICAL AND MATHEMATICAL RESEARCH

1. Approximation of Functions

Work in this area has been particularly fruitful in the past year. New approximations for the exponential integrals E_1 and Ei, and for the function e^{-x} with applications to heat conduction problems have been developed, and corresponding computer routines written. Current projects include the generation of approximations for Dawson's integral and for the Coulomb phase shift, and further development of the method of artificial poles for handling nearly degenerate rational approximations.

2. Numerical Methods in Functional Analysis

The application of the theory of complex variables to the construction of numerical methods and algorithms is continuing.

Methods for finding zeros of analytic functions, for numerical differentiation, and for numerical quadrature based on complex function evaluation have been developed and found to compare favorably with corresponding classical methods and algorithms. It is hoped that the application of the same theory may lead to computational methods for integral and differential equations; an extended investigation along these lines is envisioned.

Other research projects have been in the areas of multidimensional quadratures, of various special aspects of numerical quadrature (e.g., improvements in the adaptive Simpson method have been devised), and of calculation of Fourier and Taylor series coefficients.

3. Computation of Square and Higher Roots

Square roots on a digital computer are almost always extracted by repeated and rapidly converging improvement using Newton's method on an initial approximation of the root. For this approximation the procedure is to assume a form — a constant, linear, or rational function, for example — and to adjust the parameters of the form to produce a "level" or "best" error curve over the given range. Such a curve is one that oscillates with constant amplitude, so that the largest error is as small as possible.

It is known that a fit having best relative error at any stage of the Newton iteration process may be found by carrying the unknown parameters through one step of the process before determining their values. This complicates the equations that must be solved for these parameters. It has now been shown that this complication can be avoided by considering the logarithmic error $\hat{\delta}$ instead of the relative error δ, the two being related by $\hat{\delta} = \ln(1+\delta)$. With logarithmic error, no iterations are necessary to determine best parameters, yet these parameters remain best after one or any number of iterations, regardless of whether logarithmic or relative error is the criterion used in deciding on goodness of fit.

Furthermore, a generalized logarithmic error function has been developed for use in computing m-th roots. Again it yields a best fit for a given form without requiring any Newton iterations. Explicit formulas have been derived for the optimal initial linear fit.

4. Hydrodynamic Stability

In the study of viscous, incompressible fluids, it is necessary to know at what point steady laminar motion becomes unstable. Work has been concerned with theoretical studies of the instability of parallel shear flows. The latest work involves spiral flow between rotating cylinders. Linear hydrodynamic stability theory has been used and asymptotic solutions for large Reynolds numbers have been computed numerically from the relevant ordinary differential boundary-value problem.

Much of the effort today in linear hydrodynamic stability problems has relied upon numerical integration of the boundary value problem without any use of asymptotic analysis. The methods employed have been either initial-value shooting techniques or finite difference matrix eigenvalue methods. All such methods have difficulty at large Reynolds numbers due to the singular perturbation nature of the problem. Work has begun on a comparison of the various numerical techniques with recent improvements in the asymptotic methods. In particular, the ordinary differential boundary-value problem for the difference between the first-order asymptotic solution and the exact solution is to be solved numerically. This problem should be well behaved and should reveal to what extent the newer numerical methods can be relied upon to replace the more difficult classical asymptotic methods.

It is anticipated that the results of such a study will be used to carry out a linear stability analysis of thermal convection in the presence of a shear flow. This problem is related to studies of the dynamics of the boundary layer in the lower atmosphere and upper ocean.

5. Numerical Inversion of Toeplitz Matrices

Many problems of mathematical physics, statistics, and algebra lead to the necessity of finding inverses of finite Toeplitz or Hankel matrices. Problems involving convolutions, integral equations with difference kernels, least square approximations by polynomials, and stationary time series are well-known examples. Although there is an abundant literature on the mathematical properties of Toeplitz matrices, there seem to be only a few references to the problem of numerical inversion. The efficiencies of numerical methods involving Toeplitz or Hankel matrices are often judged under the assumption that the inversion of a Toeplitz matrix of order n requires of the order of n^3 multiplications. A new method (described in ANL-7440) accomplishes the exact inversion problem simply, using of the order of n^2 multiplications. The algorithms which were developed appear to be the most efficient ones in existence. They have also been extended to the case of vector Toeplitz matrices.

Although it was known that the algorithm might break down in certain cases, no criteria for telling when the algorithm would work were originally given. It has now been found that, assuming exact arithmetic, the algorithm will break down if and only if at least one of the principal determinants is zero. Thus the class of matrices for which the algorithm works includes the important class of positive definite Toeplitz matrices.

6. General Root-Powering Methods for Finding Zeros of Polynomials.

Earlier work in this area led to the conclusion that the general root-powering procedure for separating zeros of polynomials can be accomplished by the method of partitioning of polynomials and its algorithm described simply by a circulant representation with partitioned polynomials as elements. In an enlarged Argonne report (ANL-7344) the connection to the theory of resultants has now been shown, and an even more efficient algorithm derived for the general root-powering problem. Further investigations have shown that the problem actually reduces to that of solving a system of linear equations. In spite of the large order of the matrices, their special form permits the construction of simple algorithms which solve the entire root-powering problem in only pn^2 multiplications, where n is the order of the given polynomial, and p is the index of the transformation. These algorithms may be applied for odd values of p and for multiprocessor computer codes.

7. Generalized Midpoint Rule for Numerical Integration

The repeated midpoint rule for numerical integration is desirable both because it is simple and because it does not lead to large round-off errors. An improved generalization of this formula now permits exact integration of all first-order polynomials for arbitrary non-negative weight functions.

The problem of evaluating the integral

$$I = \int_a^b p(x)f(x)dx$$

for a given normalized weight function p(x) is attacked by first determining once and for all a set of arguments a_i as functions of p, and then approximating I by

$$\frac{1}{N}\sum_{i=0}^{N-1} f(a_i) .$$

Not only are the function values $f(a_i)$ equally weighted, but also the error of the approximation can be estimated from the second derivative of f. Errors in previously known formulas require knowledge of even higher derivatives.

8. Radiation Damage Study

The study of radiation damage from heavy energetic ions in an infinite medium consisting of atoms of only one species leads to a rather complicated system of mathematical equations. The equations can be solved separately if done in the proper order. Each equation is an integral-differential-difference equation. The equations are further complicated by the fact that the kernel in the integral part of the equation is singular. Numerical techniques for solving these equations are being investigated.

9. Infinite-Dimensional Representations of Real Semisimple Lie Groups

In the study of unitary representations of real semisimple groups, it has been known for some time that it is useful to consider a class of representations more general than the unitary ones — namely, the quasisimple representations on a Banach space. For a technical definition see (1) Chapter 1. Roughly speaking, these representations correspond to right translations on space of solutions of invariant differential equations on the group. This point of view may be thought of as a direct generalization of the theory of spherical functions. In case G is a connected real Lie group with a finite center, a fundamental result of Harish-Chandra shows that G has a "large" maximal compact subgroup K. The term "large" here means that the restriction to K of every quasisimple representation of G decomposes into a direct sum of inequivalent finite-dimensional representations of K. It should be noted that every irreducible unitary representation of G is also quasisimple. Hence the classification of quasisimple representations may be viewed as a first step in the classification of unitary representations. The problem of sorting out those quasisimple representations which are equivalent to unitary ones is treated in some detail in (2).

In (1) it is shown that every irreducible quasisimple representation is a subrepresentation of certain "standard" representations. These representations are induced representations, induced by finite-dimensional representations of certain minimal boundary subgroups. The latter subgroups are semidirect products of a maximal solvable subgroup S and a compact subgroup M. These representations are defined in a space of functions defined on the homogeneous space $M\backslash K$ and taking values in the finite-dimensional vector space on which the given representation of SM acts. For a large class of unitary representations it has been known for some time that these standard representations are irreducible. It has also been known for a long time that certain singular cases exist when the standard representations fail to be irreducible. This situation occurs, for example, whenever the standard representation contains a finite-dimensional representation. A complete discussion of this situation is given for $G=SL(n,R)$ in (1), for an arbitrary integer $n \geq 2$.

The techniques used in that discussion have been generalized further for an arbitrary simple group in (3). The situation can be described as follows. Let ℓ be the rank of the symmetric space $K\backslash G$. Then there exists a set of ℓ-proper closed subgroups of G each containing the boundary subgroup SM. Let us call these subgroups $G_1,\ldots,G_\ell$. Since each of these subgroups contains the subgroup SM, it follows easily that each vector function on $M\backslash K$ gives rise, by restriction, to a vector-valued function on $G_i \cap K\backslash K$ $i=1,\ldots,\ell$, and the set of such restrictions gives rise to an induced representation of G_i. Now, it is shown in (3) that if the standard representation is irreducible, then each of these restricted function representations of G_i is irreducible, and conversely, if each of these restricted function representations is irreducible, the standard representation of G is irreducible. The techniques used in the proof of this result enable one to construct all the irreducible subrepresentations of the standard representations in terms of irreducible representations of the subgroups G_i. For example, the degenerate series of representations correspond to the cases when some of the restricted function representations are one-dimensional.

References

1. a) E. Thieleker, Some infinite dimensional representations of real Lie groups, Ph.D. Thesis, Dept. of Math., University of Chicago, 1968.

   b) ____________, Some infinite dimensional representations of real Lie groups, submitted to Memoirs of the American Mathematical Society.

2. ____________, On the unitary representations of reductive Lie groups — applications to the real general linear group, submitted to American Journal of Mathematics.

3. ____________, The irreducible quasisimple representations of real simple Lie groups, to appear.

10. Overestimation of Entropy

It is desirable to be able to estimate the entropy of a random variable which can have K values on the basis of N samples. An efficient communication channel constructed for transmission of the values of the random variable (assuming the ergodic hypothesis) will fail if the entropy estimate is too low. Thus we wish to overestimate the entropy.

The expression of Miller and Madow for the bias of their maximum likelihood estimator has been shown to be an asymptotic expansion. Calculations have indicated that three terms of this expansion produce a relative error of less than one percent for $N \geq K$ in the case of equal likelihood. In order to use the asymptotic expansion when $N < K$, it is proposed to add K samples, one of each possible type, to the N samples. This is equivalent to the extended Laplacian estimate of probabilities.

11. Writing Projects

E. H. Bareiss and I. K. Abu-Shumays have contributed a chapter entitled, "On the Structure of Transport Operators in Space" for the book "Transport Theory," published by the American Mathematical Society in its Applied Math. Series (1968), with I. K. Abu-Shumays, Garrett Birkhoff and Richard Bellman as editors.

E. H. Bareiss will contribute a chapter to the forthcoming book "Computers and Their Role in Science," to be published in 1969, with editors A. H. Taub and Sydney Fernbach.

Two chapters, "One-Dimensional Diffusion Theory," by M. K. Butler and J. M. Cook, and "Mathematical Foundations," by J. M. Cook, were written for the book "Computing Methods in Reactor Physics" (Gordon and Breach), published in 1968. Harold Greenspan was one of the book's editors (others: C. N. Kelber and D. Okrent).

Work by J. E. Moyal and P. J. Brockwell is continuing on the book "Stochastic Transport Theory."

COMPUTER UTILIZATION IN DIVISIONAL RESEARCH

1. The Argonne Reactor Computation System

A new facility has been developed for the Argonne Reactor Computation system (ARC). It has the capability of linking modules at the time of execution, thus reducing the machine time needed to effect changes in the program modules. Hence program development time in general is reduced. Another feature provides for input card modifications without the need to respecify the entire set of input cards. Hence multiple problems can be executed easily. Furthermore, there is now an input processor with standardized and minimized input procedures for all neutronics calculations.

In production status are capabilities for one- and two-dimensional diffusion theory calculations (these include criticality and source calculations, and compositional reaction summaries); for similar calculations based on transport theory; for fuel cycle calculations, including internal and external fuel management (utilizing one- or two-dimensional diffusion theory); for input processing in fuel cycle calculations; for cross section generation (producing multigroup isotope cross sections from fundamental data).

Current efforts involve capabilities for two-dimensional transport theory, for one-dimensional synthesis based on diffusion theory, and for adjunct features involving detailed reaction summaries, perturbation, and group collapse. (See also under APPLIED PROGRAMMING.)

2. A Computerized Information and Computation System for Environmental Studies

Two basic requirements of environmental studies — (1) the retrieval of data from a large file, and (2) the application of statistical analysis techniques to the extracted data — have now been incorporated into a new computer system.

The most important criteria in developing this system were:

(1) that the data file should be structured so that data from new sources could be easily incorporated;

(2) that the system should be flexible so that any piece of data (variable) in the file could be referenced in combination with any other variable or collection of variables;

(3) that the system should be easy to learn and operate, even for those previously unfamiliar with computer applications.

All of these criteria were met in part by assigning a unique eight-character name to each variable in the data file. This name, which is presumably chosen to convey immediately the meaning of the variable, then serves as an identifier for inserting the variable into the file, for retrieving it from the file, for inserting it into a computational routine, and for displaying it in printed or graphical form.

The system contains several file structure and maintenance programs for the purposes of converting new data to the data file format, assigning names to variables, merging new data into the file, and so forth. Once the data file has been constructed, a data retrieval package is invoked through the use of a pseudo-language. This easy-to-use language extracts the variable name from an input card and uses it to retrieve the desired variable from the file.

Computationally, the system contains a multivariate regression analysis package and a stepwise discriminant analysis program. In addition, a number of other routines for adding data to the file, operating on data, or displaying data have been developed. The system has been so constructed as to allow these routines to be added in a straightforward manner. Thus, it is expected that the system will continuously increase in capability through the contributions of those using it.

Although general in concept, this system was created for use by the air pollution prediction modeling effort at Argonne National Laboratory, and it has proved quite useful in support of this project.

3. Living Cell Measurements

The possibility of making measurements of the motility of living cells in vitro is of considerable scientific interest for two reasons. In the first place, it is known that different cell types may have different characteristic levels of activity. For example, malignant cells may appear more active than normal cells of the same kind. Secondly, on the basis of information concerning the average motility of a known cell type, it may become possible to evaluate the influence on motility of such factors as temperature, oxygen tension, pH, or action of different chemicals or drugs introduced into the medium. Consequently, a working system for quantitation of cell movement in vitro may supply a remarkable tool for pharmacodynamic studies on the cellular levels.

The technique outlined in a recently submitted paper* consists in analysis of sequences of time lapse photographs of single living cells, using the CHLOE film scanner to transform the photographs into digital form. By mathematical methods previously developed for chromosome spread analysis, each instantaneous cell configuration is represented by a single point in a 7-dimensional measurement space. The cell motion then maps into a trajectory in this space, and the length of the trajectory is used as a measure of cell movement.

The figure shows a photograph of original views and digital reconstructions of three types of cells used in the study. Number 554 is a subcutaneous mouse tissue fibroblast maintained in a "starved" state to serve as a dead control; No. 560 is a liver macrophage from a fragment of newborn mouse liver; No. 540 is a peritoneal macrophage from an adult mouse.

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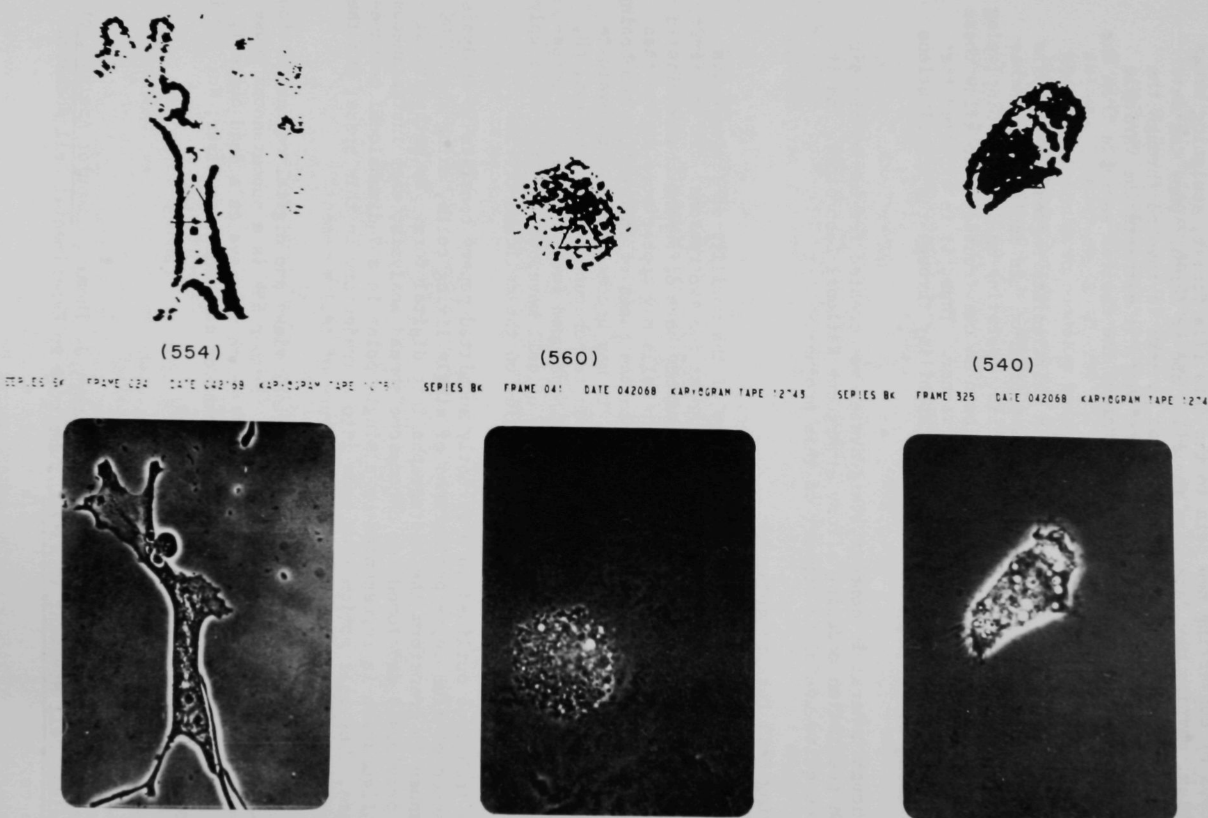
*Georges Barski, J. W. Butler, and Robert J. Thomas, Computer Analysis of Animal Cell Movement in Vitro, submitted to Experimental Cell Research.



The Figure Shows a Photograph of Original Views and Digital Reconstructions of Three Types of Cells Used in the Study. Number 554 is a subcutaneous mouse tissue fibroblast maintained in a "starved" state to serve as a dead control; No. 560 is a liver macrophage from a fragment of newborn mouse liver; No. 540 is a peritoneal macrophage from an adult mouse. (ANL Neg. No. 145-1094 Rev. 3)

4. Random Number Generation

Often the most convenient mathematical model for a physical or biological phenomenon is statistical, especially (but not necessarily) when our intuitive picture of the phenomenon is already naturally statistical, as is the case with neutron transport.

Computations based on such models require a source of numbers capable of passing certain tests for "randomness." It has been customary to use algorithmic schemes for producing these numbers, but recent theoretical results [G. Marsaglia, Proc. Nat. Acad. Sci. 61 (1968), p. 25] have confirmed suspicions arising from a growing body of empirical evidence that these schemes have serious defects. Since it is of fundamental importance that a good source be available, a return to the older physical (non-algorithmic) methods is indicated.

A solid state random bit generator manufactured by Burrbrown Co. is soon to be attached to the Applied Mathematics Division's IBM-1130 computer. It generates a random 0 or 1 whenever it is fed a clock pulse, up to a rate of one megacycle. Bits will be combined to given random 12-bit numbers that will then be recorded for later use. This will make computational results based on these random numbers reproducible.

A scheme based on the use of radioactive decay has been devised by N. Frigerio of the Biological and Medical Research Division, and other schemes using pure quantum noise are being considered. A number of people at the Laboratory have interest and experience in the generation, testing, and use of random numbers. Paul Benioff of the Chemistry Division is working on the metamathematical aspects of the notion of randomness.

5. Supersonic Gas Flow Computations

A very general computational scheme for plane supersonic gas flow through ducts and around obstacles has been developed during the past several years. Its accuracy mainly depends, in a particular case, on whether the assumption that viscous and heat-conductive effects may be confined to oblique shocks is justified. Oblique shocks are those represented by abrupt changes in flow variables.

The numerical techniques used include Hartree's method of characteristics, shock-fitting procedures developed by Zhukov and Moe-Troesch, and Powers' use of the stream function for accurate calculation of entropy. Features of the scheme are that it will keep track of an arbitrarily large number of discontinuities and will introduce those shocks, vortex sheets, and midflow expansions necessary to represent discontinuity interactions.

Specification of the flow at the inlet (upstream) end of the duct provides primary boundary conditions. A variety of secondary boundary conditions may be prescribed by the designer of a supersonic intake or nozzle: the boundary streamlines (walls of the duct) may be specified by their position, by defining the values of some fluid dynamic variable on them, or by requiring that they produce a Mach line focus at a specified point.

The methods used are applicable to the calculation of weak solutions of other hyperbolic systems, and the scheme could be extended to include boundary layer effects.

6. Automatic Theorem Proving

The ground work for a general theory of inferentially general inference systems has been formulated. Inferentially general systems involving inference rules such as paramodulation and resolution appear to be the most effective known bases for computer-based automatic theorem proving and general question-answering systems.

Proofs of the logical completeness of paramodulation for functionally reflexive first-order theories with equality (e.g., basic group theory) and a presentation of some of the concepts of the theory of compact systems were given recently in a paper at the Fourth Annual Machine Intelligence Workshop in Edinburgh. This paper will appear in Vol. IV of Machine Intelligence. From the viewpoint of efficient computer theorem proving this new completeness result is an improved strengthening of results previously published in the Journal of Symbolic Logic.

The research project in theorem proving is a joint effort of Argonne and the Stanford Linear Accelerator Center.

7. Reactor Mathematics

Development and research work in reactor mathematics in the Applied Mathematics Division is at present primarily concerned with transport theory and flux synthesis.

In the case of transport theory, the primary goal is the development of an effective two-dimensional multigroup transport algorithm as a part of the ARC (Argonne Reactor Computation) system for the IBM S/360 computer. The main constraint on this project is the need to develop an algorithm capable of immediate production use. With this constraint in mind, the main structure of the algorithm will be based on the S_n approach, including the same spatial differencing that was involved in the CONTROL DATA 3600 codes. Within this basic structure the main areas of research and development include the following:

(i) The algorithm has four levels of iteration. The structure of the matrix involved in the innermost level is being investigated in order to determine an effective acceleration algorithm for use at this level.

(ii) The speed and sensitivity of the second level of iterations is being investigated with a view toward the possible inclusion of an acceleration procedure at this level.

(iii) A data scheme being developed for this algorithm is based on the configuration and capabilities of the present computer. Thus, for example, the use and interrelation of disks, large core storage, and fast memory with regard to this algorithm is being investigated.

(iv) Somewhat longer range goals include the development of an alternative approximation which aims at correcting at least two major faults of the present algorithm. Namely, 1) the production of negative (hence physically meaningless) fluxes in some cases, and 2) the disjointed structure of the four levels of iteration; this makes for difficulty in designing acceleration procedures.

The second major effort is in the area of flux synthesis. In this case the immediate goal is less production-oriented than the transport goal. The present effort is involved with developing an algorithm for two-dimensional static flux synthesis from one-dimensional fluxes. This is a joint Reactor Physics-Applied Mathematics Division effort, and the investigation is proceeding at several levels. At the variational level there are two functionals being studied. Numerical approximations for each of the resulting Euler equations are also being developed. In addition, data management schemes for the resulting algorithms must be constructed.

Other efforts in the latter stages of completion include final testing, adjusting, and experimentation for

(i) the two-dimensional multigroup diffusion theory algorithm;

(ii) the high-order finite difference algorithm based on Hermite interpolation for the Sturm-Liouville problem;

(iii) the particle transport code for slab geometry based on the stochastic model with the icosahedral direction approximation.

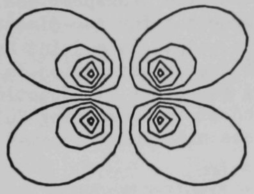
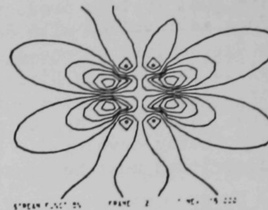
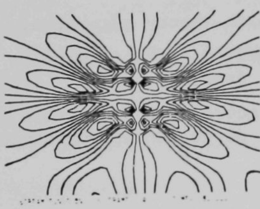
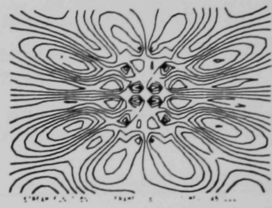
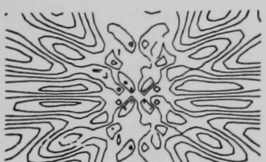
8. Perturbation Collapse in an Infinite Ocean

The question of what happens when a source of perturbation is introduced into a large body of water is of fundamental interest for oceanographic studies. Recently a flexible computer program for solving hydrodynamic equations describing the propagation of an oceanic perturbation has been written; it takes into account density variation, heat conduction, and viscosity.

The initial perturbation is treated as the mixing of a small quantity of fluid at the center of a large rectangle in an infinite two-dimensional ocean of fluid that has an initial density gradient depending only on depth. The mixed fluid begins to spread out as soon as it is released.

The program output is in the form of tables of numerical values and 35mm film images produced at intervals during the computation. The film images are "snapshots" of what is happening to lines which represent constant fluid density and give a total picture that can be evaluated easily. Particularly interesting are the pictures which show the generation of internal waves in the large body of fluid as the area of the mixed fluid collapses. An 8mm moving picture has been made from one "run" of these 35mm film images and shows the collapse of the perturbation and the spread of internal waves with almost exactly the same details as moving pictures made of corresponding laboratory experiments.

The program has been very successful in duplicating the general physical behavior of laboratory experiments, including some with non-linear and even discontinuous density variation. It will also be used to study convective overturn due to surface cooling by application of the numerical methods developed so far to an ocean with a free surface undergoing heat loss. Oceanographers are interested in the onset and development of the downward convection which arises from the cooling of the ocean surface by conduction, radiation, and evaporation. If successful, this approach should make it possible to observe numerically such effects as the development of the plunging sheets of cooled water reported by Spangenberg and Rowand and the development of the well-defined convection cells reported by other investigators.

These pictures were produced directly on film by the CDC 3600 computer in the course of a two-dimensional hydrodynamics calculation. The calculation describes the behavior of a region of fluid that initially has a constant vertical density gradient everywhere except in a square sub-region where the fluid has been uniformly mixed. Shown in these pictures are streamlines at successive time intervals during the collapse of the square region of mixed fluid. Time is given in seconds, and the Väisälä-Brünt frequency is $w = .25\ \sec^{-1}$.

9. Cell Population Growth

Various mathematical models for cell population growth have been derived and are now being tested against experimental growth curves. The experimental growth curves exhibit an "overshoot" before leveling off to a constant value. This excludes models which have the semi-group property.

COMPUTER ENGINEERING RESEARCH AND DEVELOPMENT

1. Mössbauer-Effect Data Collection System

This system, utilizing a small digital computer with interface, has now been installed in the Physics Division. It was developed to gather data from four Mössbauer-effect experiments simultaneously, to provide a display feature, and to output data onto paper tape.

Results are very gratifying in the accumulation, control, and display areas. The control program gives the experimenter great flexibility by allowing him to enter various commands and parameters from the typewriter. Options include the initiation or deactivation of any of the experiments, display of any portion or all of any of the experiments at fifteen different scale factors, and binary-to-decimal conversion for output on either the typewriter or the paper tape punch.

Much of the effectiveness of this system is achieved by performing the additive functions for channels in the interface hardware. This feature permits a rapid and meaningful display under program control and even permits data accumulation when the computer is in a "halt" condition.

The system as it now functions is considered fully operational. The failure rate of the computer and its interface is excellent, surpassing that of the multichannel analyzers it has replaced. No major changes in the system are now contemplated. However, an addition to the hardware to permit a higher resolution calibration function for each of the experiments is planned. Furthermore, software modifications will, of course, be made as required and desired.

2. Nuclear Emulsion Scanning System

The goal of this project is to provide, in a joint effort between the Physics and Applied Mathematics Divisions, a fast, computer-controlled scanner that will automatically count the tracks of charged nuclear particles on fine grain emulsion plates exposed in a magnetic spectrograph. This scanner, utilizing a commercial image dissector as the scan tube, has now been refined to the resolution limits of the image dissector.

Such automatic scanning of nuclear emulsion plates has led to development of controlled procedures for plate handling and plate development. The result of this effort has been the production of low-noise, high-contrast plates.

At present (late 1968) the counting efficiency of the scanner is approximately 90% in high track density areas, where tracks tend to blend into each other, and nearly 100% in lower track density areas. This loss of counting efficiency in high track density areas reflects the limited scan tube resolution. A new tube has been evaluated and found to be able to resolve 3 microns in the emulsion; this is the approximate resolution of the imaging lens. The incorporation of the new scan tube, presently in progress, will raise the counting efficiency in high track density areas to approximately the same efficiency as that in low density areas, and thus permit the automatic processing of all subsequently produced nuclear emulsion plates.

3. Computer Control of Diffraction Equipment

The practicality and economy of small digital computers have led to their increased usage in controlling certain pieces of experimental apparatus. Such a computer is a vital part of the ARCADE system — an on-line, computer system used to control experiments and collect data in both neutron and X-ray crystallography according to predetermined algorithms and to feed data back from the experiment.

There are three ARCADE systems now in use at Argonne's CP-5 reactor; the first controls a full circle goniostat (crystal orienter), the second a heavy-duty spectrometer and cryo-orienter, both for the Metallurgy Division; the third system controls a polarized neutron diffractometer for the Solid State Science Division. A fourth system has been integrated with a General Electric quarter circle X-ray diffractometer at and for the Chemistry Division, while a fifth, being developed by the Electronics Division, will control a full circle X-ray unit for the Biology Division. All of these systems utilize IBM 1130's as control computers.

A large array of user programs for the ARCADE system have been developed. As an example, the basic crystallographic programs provide:

1. Routines whose input parameters describe the current experiment.
2. Least squares programs to determine the lattice and instrument constants.
3. Data collection programs which generate d-spacings and instrument angles under various options and perform automatic step scans of peaks.

The flexibility and reliability of the system provides the experimenter with a system which is convenient to operate and increases the quantity and quality of data obtained.

4. Remote Access Stations

The Remote Access Data System (RADS) is a digital computer system which allows remote entry of jobs for batch processing in the IBM 360 computer. Remote stations, located in various buildings at Argonne, will communicate over telephone lines with a centrally located Message Switching Computer, MSC, which will in turn communicate with the IBM 360 system through an IBM 2701 Data Adapter unit.

The remote stations will be built around Varian Data Machines 620I computers, G.D.I. (General Design Incorporated) card readers and Potter line printers. Future developments call for the addition of various types of peripheral equipment such as card punches, paper tape input/output devices, and so on.

Hardware and software development for the initial phases of the system is well under way. Jobs have been entered remotely, scheduled by the 360/50, run on the 360/75 (which operates in tandem with the 360/50), and printed remotely using a single remote station. The next phases of development call for the installation of the system in the production version and the building of multiple stations.

Special integrated circuit boards have been designed and are being built for the remote stations. The entire controller for a single device such as a card reader, paper tape reader, printer, or transceiver can be placed on a single board, thus reducing backboard wiring and the added expense of multiple boards. An automatic wire wrap procedure for the integrated circuit boards is used because it (1) reduces the time to get boards wired, (2) produces a much more accurate system, thus reducing the time required for debugging, and (3) reduces manpower requirements and hence cost per board.

At this time (Fall, 1968), six remote stations are at some phase of completion, with a possibility of more in the future. Controllers have been designed, built, and tested for the card reader (600 cards/minute), the paper tape reader (625 characters/second), the telephone line transceiver (5000 bits/second), the line printer (300 lines/minute), and a Calcomp plotter (300 steps/second).

For expeditious testing of equipment to be used at the Remote Stations, a general-purpose controller has been built and is now being used on an incremental magnetic tape drive. The tape unit selected was the Peripheral Equipment Corporation's (500 bytes per second) incremental write and (10,000 bytes per second) synchronous read device. The program which exercises the magnetic tape unit has just been completed and the unit is now undergoing tests; the first indications are good. The interface for the Calcomp has been completed and tested, but the final software has not yet been written.

The desirability of having printers operating at 1000 lines per minute has inspired tests on the telephone lines to determine if the data rates could be increased from 5,000 bits per second to 20,000 bits per second. This data rate seems possible but further tests must be made with complete transceivers and computers on each end.

5. Braille Reader

Work is starting, in part under a contract with the Department of Health, Education, and Welfare and in association with Arnold P. Grunwald of the Reactor Engineering Division, on a Braille reader for the blind. This unit, when finished, will consist of a small, low-cost package containing an audio magnetic tape playback unit, a Braille media belt and transport, and associated electronics.

Written or spoken information stored on audio tapes as properly formatted Braille characters will be converted into embossed symbols on a reusable plastic belt loop which can then be read by the user. Movement of the magnetic tape and Braille media belt will be synchronized and controlled electronically. Embossing speed, direction, and skimming will be continuously variable and under control of the user.

At present, working electronics and mechanics for a first "breadboard" is near completion, and design is beginning on a more advanced system.

A means will be provided to translate written information into Grade II Braille and to put this Braille code onto magnetic tape with proper formatting. Because of contractions and contextual dependence, Grade II Braille translation is highly nontrivial. Work is beginning on the conversion of an existing translation program into the PL/1 language for use on IBM 360 computers.

6. Opto-electronic Information Storage

A research project to determine the feasibility of storing binary information on photographic plates utilizing holographic* techniques has been in progress for some time. The initial goal is to store a 64 x 64-bit (binary digit) array of information in a holograph 2mm on a side. A 64 x 64 array of such holographs will be placed on an emulsion-covered glass plate, thus yielding a total information storage capacity exceeding 16 x 10^6 bits per plate. Since the process of storing information on the plate will consume a considerable amount of time by computer standards, the projected use is for read-only storage, e.g., assemblers, compilers, archival material. It is estimated that the writing and development will take approximately four hours.

An automatic movable stage has been designed and is being constructed for the preparation of fully populated holographic plates. This stage, consisting of beam splitters, mirrors, spatial filters, and beam expanders, will permit the exposure of holograms over the entire photographic plate surface in such a manner as to place all the image reconstructions in the identical position in space.

Reading the stored information will be accomplished by utilizing a single detector array and switching the illuminating laser beam to the various holographs by means of a series of opto-electronic switches and bi-refringent crystals. With this technique it should be possible to select any of the holographs in the array in approximately four millionths of a second. Several switch and bi-refringent deflection stages have been ordered. These initial stages will permit the evaluation of the drive electronics already prepared and will also permit an evaluation of the actual optical properties of the crystal as well as the associated index-matching fluids.

Once a holograph has been selected and illuminated, its 4096 bits would be available in parallel. Utilization of the information can then be governed by conventional electronics. Several experimental photodetectors have been evaluated and have been found capable of detecting the individual information bits. The problem of packaging a 64 x 64 array of photodetectors remains to be solved.

An optical bench to eliminate the effects of building vibration has been constructed. Its relative vibration limitation is on the order of 1000 Angstrom units.

A number of holographs — both of the reflected light type and of the direct transmission type — have been prepared. Efforts are currently being directed toward higher efficiency holographs of the desired storage density.

Holographic memories have great potential because they not only provide large storage capacity but also imply high reliability due to their redundancy.

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*A holograph is a photograph of a three-dimensional diffraction pattern.

7. Pattern Recognition Research

A. Fingerprints

A program is being developed to extract ridge-endings from a fingerprint pattern in the presence of noise. The approach taken is to generate a node table that includes all the ridge-endings plus many false nodes. Through a process of combining nodes and deleting them, the table may be reduced to one containing only legitimate ridge-endings. It appears that this approach will locate about 90% of the ridge-endings, although about 20% of the remaining nodes will be false. Work is continuing in an effort to improve the approach. A list-processing scheme is now being tested; results are encouraging.

This work was published in a report to appear in the proceedings of the Second National Symposium on Law Enforcement Science and Technology. A paper entitled "Machine Classification of Fingerprints" is to appear in Argonne National Laboratory Reviews this year. Argonne's Science Radio Series contained an interview entitled "A Computer Looks at Fingerprints." This series is being broadcast by over 800 radio stations throughout the world, including the British Broadcasting Corporation.

B. The Visual Fields Problem

A preliminary study has been made of the visual fields problem, and a research proposal is to be prepared with the assistance of Dr. Tibor Farkas of the Department of Surgery (Ophthalmology), University of Chicago.

The correct interpretation of abnormal visual fields is a powerful technique for an early detection of diseases affecting the visual pathway. There are two areas where digital techniques and pattern recognition might make a contribution. First, the visual field patterns may be digitized in such a manner that they can be stored, along with other medical records, on magnetic tape. They may later be recalled and viewed on a graphic display device. A program for displaying visual fields has been written for the IBM System/360 Display Unit (2250). Second, using pattern recognition techniques, the abnormal visual field may be categorized. Operating in this mode, the system could act as a digital reference manual.

8. Film Scanning (ALICE Project)

Development work has started on a new general-purpose film scanning device (ALICE) that is to take advantage of improvements in cathode ray tube technology and of the much faster control computers now available. ALICE is to be more accurate, more versatile, and five to ten times as fast as the present CHLOE system. Its two major elements will be a commercial digital computer with magnetic tape and an Argonne-built cathode ray tube scanner.

Although CHLOE has proved quite useful in a wide variety of applications, potential improvements that could be implemented in ALICE include:

1) Input facility for varied types of film material.
2) Increased resolution.
3) More accurate discrimination among shades of gray.

4) Rotational capability for input.
5) Color discrimination.
6) Flexibility in man-machine interaction.
7) Higher level programming language.
8) Several input stations, including a reflected light scanner.

It is planned to pay significant care to the light measuring capabilities of the equipment so that stable, reliable optical film density measurements can be made. Furthermore, some use is to be made of analog deflection systems to allow for less accurate but very fast searching for information to be digitized.

Initial effort is directed toward means of cathode ray tube intensity control that would allow discrimination of as many as 64 different shades of gray. Furthermore, the feasibility of a reflected light scanner has been demonstrated; this was accomplished using the CHLOE system but repositioning its photo detectors.

An attempt is being made to design equipment useful in other programs at Argonne, and in particular to plan for processing film material containing biological data.

9. Hybrid Computing

Certain classes of problems lend themselves to digital solution while others are handled more readily by analog computers. An optimum solution to many intermediate problems can be accomplished by combining both types of computation into a single hybrid system, and this is now being done in the Applied Mathematics Division.

One example of the type of problem to be handled is the analysis of feedback control systems. Either analog or digital methods alone could be used, but each has pronounced shortcomings in this kind of problem. A digital solution alone would be very expensive in both programming and machine time. On the other hand, an excessive or even prohibitive amount of equipment would be necessary for an analog solution.

The analog facilities in the Applied Mathematics Division consist of two Pace consoles and two Reeves consoles. These analog consoles were previously interconnected through an appropriate hybrid link to a small digital computer as an earlier hybrid system. The present system, which is soon to become operational, uses the more powerful IBM 1130 as the digital computer.

The 1130, delivered in June, has been operational since its arrival. It features a disk monitor system and a card reader-punch; the latter will be useful for other 1130 computers at the Laboratory — none of which have such a device. Since this computer serves as a focal point for the 1130 programming effort at the Laboratory, the anticipated work load was heavy enough to warrant the addition of a line printer and an extra portion of magnetic core memory, both now on order. The line printer will speed output operations by a factor of 15 to 20, while additional memory space will eliminate the frequent need to fragment programs during their execution.

10. Computer Associated Interactive Graphics

A study has been initiated in the area of computer associated interactive graphic systems. Systems of this type provide a means for man/computer dialog (interaction) using graphs and pictures as well as written information.

Presently there is much activity in the area of graphic data processing. Several high-level programming languages have been prepared, and a number of graphic terminals, both experimental and commercial, have been proposed and built. The growth of time sharing computer systems has added its impetus; it is in this type of system with its dialog capability that interactive graphics seems to be used most advantageously.

The results of investigation to date indicate some desirable properties: 1) An operator should be able to manipulate parts of a display without affecting the display as a whole. 2) The display should also be able to attract the user's attention. 3) Scale changing is necessary. 4) The user must be able to attach labels and values to the various items of a display. These labels and values must not only be associated with the item in the user's mind but also must be associated with the item in the machine. 5) It would be desirable to minimize the amount of pointing necessary to "talk to the display."

Looking at methods by which these features as well as others may be implemented suggests that a list processing capability, associative data structures, and large memories are desirable if not necessary.

One possible approach has been partially worked out. A small associative list machine language and a hardware list processor have been outlined. A single multihead magnetic disc memory is proposed to handle all memory requirements and a TV-type display with interactive capability has been shown to be workable.

Investigation is continuing into further systems aspects and other approaches to implementation.

APPLIED PROGRAMMING

The Applied Programming Section consists of four groups, whose organization is based on functional demarcation; namely, Theoretical Physics and Chemistry, Experimental Science, Reactor Theory and Development, and Engineering and Applied Systems. Following is a brief summary of the work of each of these groups.

Theoretical Physics and Chemistry

A set of programs to calculate Slater parameters, energy levels, and atomic spectra has been written. Fitting of up to 30 parameters simultaneously involved in fifteen 100 x 100 energy matrices can be done.

The optical model program, ABACUS, has been expanded and a new program written to compute magnetic field in the design of an electron microscope.

A technique is being developed to solve the integral equations which determine the distribution of ranges of heavy energetic ions in a random infinite medium and the spatial distribution of the deposited energy (radiation damage).

Work on the reduction of group representations and development of other methods for reduction of an arbitrary representation has been continued. Representations of the cubic group using the Wigner coefficients have been devised and published.

Two large efforts completed during this past year have centered about the exploitation of the new PL/1 programming language. In one, an interface has been established between FORTRAN and PL/1. Advantage can now be taken in a PL/1 program of the large library of FORTRAN subroutines, while FORTRAN programs may now employ the bit, character, and interrupt manipulation techniques of PL/1.

In the second, a special-purpose language has been developed to facilitate easier use of least-square fitting programs. Specification of the function and gradient can be made conveniently by the user as data to a program which produces in turn the corresponding FORTRAN-language function subprogram formally required by the minimization routine. Both of these projects are described in forthcoming laboratory reports.

The Job Control Language for 360 Operating System communication has been applied in two important FORTRAN areas — the accessing of information on multi-file magnetic tapes, and the updating and editing of FORTRAN source codes. Emphasis was placed on accessing arbitrary files on the multi-file tapes with consideration given to coding requirements and tape handling restrictions. The Source Code editor provides a limited facility for changing variable names in FORTRAN source programs.

Experimental Science

A least squares fit was made to conductivity vs. temperature data of ionic crystals, and another fit was made of efficiency of a fluorine reactor. Other efforts included an analysis of fuel rod density and radioactive profiles, a calculation of stored energy in radiated materials, and performance of material balance and data reduction calculations for a fluid-bed reactor. Finally, a study was made of bubble chamber convective flow.

Reactor Theory and Development

In addition to those items concerning the Argonne Reactor Computation system (ARC) discussed under COMPUTER UTILIZATION IN DIVISIONAL RESEARCH, work has been done on the following projects:

The stochastic model, multi-energy, icosahedral direction approximation particle transport code for slab geometry has been developed and used with energy-dependent cross sections. To reduce the labor of input data (cross sections) preparation in using the multi-energy code, a subsidiary code has been written to prepare the ultimate input data in the proper form, from cards containing more-fundamental and substantially less input data. Work is proceeding to add capability to compute higher moments of distributions obtained.

Other efforts within the group provided for the solution of Sturm-Liouville systems, stiff differential equations, and integro-differential equations with time lags. Programs for Fourier integral evaluation and Gauss-Legendre and Gauss-Laguerre quadrature were developed.

Work has also begun in support of the new environmental sciences effort recently initiated at Argonne; it encompasses two areas of the air pollution system model for the City of Chicago:

(1) the development of an information and computational system for use in the statistical air pollution prediction program (see details under COMPUTER UTILIZATION IN DIVISIONAL RESEARCH),

(2) the development of a computerized central model for public utilities during incidents of high pollution.

Engineering and Applied Systems

An interface within ASP (Attached Support Processor) has been programmed on the IBM 360/model 50 system to provide two-way communication to a 620I Message Switching Computer which in turn interfaces over phone lines to remotely located computers called RADS stations. Such stations permit users to enter 360 jobs remotely as well as to receive output. Current programming is functioning satisfactorily for a single station and multiple stations will be included in the next level of program development.

A number of extensions and refinements have been completed with respect to the IBM 1130 programs controlling the neutron diffractometers at the CP-5 reactor and a GE X-ray diffraction system.

A comprehensive control and data analysis program has been written for the 70-inch scattering chamber. The major milestone achieved in this system is the capability of gathering data while simultaneously utilizing a scope display equipped with light pen for on-the-spot analysis of data already collected. An ASI-210 computer to which a large bulk core memory has been attached is involved. An overlay system has been programmed using the bulk memory as the auxiliary device that holds all the segmented programs.

A fault-tree analysis program, applied to a variety of components within a nuclear reactor, is used to determine the parallel and sequential combinations of component status that can and will result upon the occurrence of a specified component event. The states are represented by a boolean expression.

An initial simplified version of a management information system is in operation. Future versions will contain more diversified facilities that will enable users to obtain a greater variety of reports.

An applications job library has been assembled and made operational on the IBM 360/System. These programs are valuable aids to the problem solver, particularly in a scientific or technical environment. Available systems currently reside on a single disk pack. Among the sets of programs included are: AUTOFLOW, a program for preparing flow charts automatically by computer using 360 FORTRAN or Assembly language source code as input; Scientific Subroutine Package, a collection of FORTRAN IV utility subroutines; PL/1 FORMAC Interpreter, an extension to the OS/360 PL/1 compiler that provides for symbolic manipulation of mathematical expressions; and Document Processing System, a system that stores keywords, abstracts, or complete text into well-organized files and provides various search strategies for retrieving document information from these files.

The following programs have been completed by the Applied Programming Section in the past year:

06E7016 COMPUTER SERVICES REPORT FOR LABORATORY ACCOUNTING

This program prepares a monthly report to the Accounting Department and to the individual laboratory cost centers, itemizing the programming time of AMD personnel and the operation time and performance statistics of the major AMD computers.

08E7037 LEAST-SQUARES CALCULATION OF VAPOR PRESSURE

The constants in the linear relationship between the logarithm of the vapor pressure and the reciprocal of the absolute temperature are determined by a least-squares method. The vapor pressure is computed from measured values of the cell parameters, corrected where applicable for thermal expansion, and experimental data of the displacement of the effusion-cell with temperature. The program corrects for nonlinearity, created by an inaccurate zero of the displacement, by seeking a minimum in the standard deviation of the isopleths found by making successive changes in the numerical value of the zero.

09E7030 MIG — MANAGEMENT INFORMATION GRAPHS

The program MIG uses the data from the Accounting Department to compute projections of the annual firm and flexible costs, which can then be printed or graphed.

11E7041 HIGH-TEMPERATURE THERMODYNAMIC FUNCTIONS (ORNL)

PLOTHEAT uses the method of least squares to fit high-temperature enthalpy data to one or several selected functions. From the generated equation, heat capacity, enthalpy, entropy and the free energy function are calculated and tabulated at 100° increments. Plots are also made of temperature versus enthalpy.

12E7039 REDUCTION OF MÖSSBAUER DATA

This program is an extension of 2151/PHY 303, Line Shape Fitting by Variable Metric Minimization. There exists an option to plot results on either the DD80 or CALCOMP 580.

17E7056-7 TWO- AND THREE-DIMENSIONAL CRYSTALLOGRAPHIC FOURIER SUMMATION PROGRAM

This program performs two- and three-dimensional Fourier summations ($\rho(x,y,z)$) for crystallographic purposes to produce Patterson, electron density, and neutron scattering density patterns, when Fourier coefficients are derived from X-ray and neutron diffraction data. An option of this program calculates coordinates and peak maximum values from the calculated maps.

19E7062 CRYSTALLOGRAPHIC D-SPACE PROGRAM

The program generates Miller indices tests for space-group extinctions, and calculates d, $1/d^2$, $\sin\theta$, $\sin^2\theta$, $(\sin\theta)/\lambda$, $(\sin^2\theta)/\lambda^2$, θ, and 2θ for any crystal system and space group, requiring only the unit cell parameters as data input. Optional output are 2θ corrections and the single crystal angle settings. (ANL-6519)

24E7075 PLUME RISE

This program is an extension of Library Program P174, which makes a linear regression calculation involving plume rise from smoke stacks.

25E7080 STATISTICAL ANALYSIS OR PARTIALLY ORDERED DEFECTS IN NONSTOICHIOMETRIC IONIC CRYSTALS

Nonstoichiometric crystals contain defects which, contrary to the common assumption of statistical analysis, are probably not randomly distributed over the eligible lattice positions. This present treatment assumes that defects of a particular kind (such as anion vacancies) repel each other from nearby sites; the number of sites a defect controls is then related to its position in a series of energy levels. The distribution and interaction energy functions arising from this model are substituted into a grand partition function for defects in a nonstoichiometric crystal.

31E7099 AVERAGING AND PLOTTING OF INTENSITY DATA

The program reads and averages intensity data and angle positions, and plots these data vs. 2 THETA or sin(THETA)/LAMBDA values off-line.

An option of subtracting the background, which may be read as the first set of data, is included.

32E7102 TOTAL ENERGY FOR EQUAL TEMPERATURE INTERVALS

This program computes the total energy for equal intervals of the temperature from experimental measurements of temperature, voltage and current.

33E7103 TEMPERATURE AND RESISTANCE CORRECTIONS FOR BOMB CALORIMETRIC DATA

Temperature and resistance corrections are calculated from bomb calorimetric data for given thermometers and bridges.

36E7118 A FORTRAN CRYSTALLOGRAPHIC LEAST-SQUARES REFINEMENT PROGRAM

The program performs the least-squares refinement on crystal structure parameters based on X-ray or neutron diffraction measurements.

This program permits 1) the use of both isotropic and anisotropic temperature factors based on the individual atom selection, 2) the choice of scaling the change of the individual parameters varied, 3) the treatment of atoms in the special positions using the input cards, and 4) the correction of X-ray data for anomalous dispersion effects. The basis of this program is MET 153.

38E7139 PIE — PHOTOIONIZATION EFFICIENCY

PIE is a program to reduce the photoionization experimental data to photoionization efficiencies or logarithms of photoionization efficiencies and then plot these computed values vs. wavelengths.

39E7144 CALCULATION OF X-RAY POWDER DIFFRACTION PATTERNS

This program calculates the positions and intensities of reflections of powder diffraction patterns using unit cell data and the atom coordinates. An option is provided to plot a simulated diffractometer chart using either Gaussian or Cauchy profiles.

43E7152 CALCULATION OF THERMODYNAMIC FUNCTIONS OF GASES

This program will produce a table of functions which correspond to Gibbs' Energy, Enthalpy, Entropy, Equilibrium constant, and others which represent thermodynamic properties of an ideal gas.

53E8187 FLUID BED REACTOR DATA ANALYSIS

This program represents the components of a fluid-bed reactor and performs material balances and data reduction calculations.

55E8194 CALCULATION OF FOURIER TRANSFORMS

Calculation and plotting of Fourier transforms for functions defined by data are done by this program.

57E8199 INTEGRAL EVALUATION

This program produces a table of values of an integral which is related to a complex error function.

58E8200 DETERMINATION OF ELASTIC MODULI AND COEFFICIENTS OF INTERNAL FRICTION

This program evaluates elastic moduli or internal friction coefficients from data punched in BCD or EBCDIC code.

61E8205 FLUORINE EFFICIENCY FIT

Variable Metric Minimization is used to fit data to a fluorine efficiency equation.

09R7047 AARR PRESSURE VESSEL CONTAINMENT POTENTIAL

This program determines the containment potential of the AARR reactor vessel and estimates the strain energy imparted to the vessel.

13R7104 SNARG1D — NO NEGATIVE FLUX FIXUP

This program processes SNARG1D (ANL-7221) runs without utilizing the negative flux fix-up option.

14R7106 AARR PRIMARY COOLANT SYSTEM CONTAINMENT POTENTIAL

This program determines the containment potential of the AARR primary coolant system and estimates the strain energy imparted to the vessel and the coolant system.

04S7007 LIBRARY DEVELOPMENT FOR S/360

ANL F402, MATINV

This program, in subroutine form, solves the matrix equation AX=B, where A is a square coefficient matrix and B is a matrix of constant vectors. The determinant and inverse of A are also obtained.

ANL C250S, CUBIC

This program, in subroutine form, finds the three roots of a cubic polynomial equation.

ANL C251S, QUARTI

This program, in subroutine form, finds the four roots of a quartic polynomial equation.

ANL F202S, EIGEN

This program, in subroutine form, finds all scalar solutions, λ_i (including proper multiplicity), and the associated orthonormal vectors, x_i, to the matrix equation $Ax=\lambda x$, where A is a real, symmetric matrix.

ANL F252S, GEIGEN

This program, in subroutine form, finds all scalar solutions, λ_i (including proper multiplicity), and the associated unit vectors, x_i, to the equation $Gx=\lambda Fx$; here G and F are real, symmetric matrices with F positive definite.

ANL F250S, FRANCI

This program, in subroutine form, finds all scalar solutions, λ_i (including proper multiplicity), to the matrix equation $Ax=\lambda x$, where A is an arbitrary real square matrix.

ANL F453S, MATINV

This program, in subroutine form, solves the complex matrix equation AX=B, where A is a square coefficient matrix and B is a matrix of constant vectors. The determinant and inverse of A are also obtained.

04S7007 LIBRARY DEVELOPMENT FOR S/360 (Cont'd.)

ANL F454S, CROUT

This program, in subroutine form, solves the matrix equation AX=B by the Crout method; here A is a square coefficient matrix and B is a matrix of constant vectors. The determinant of A is also obtained.

ANL F152S, SYMINV

This program, in subroutine form, solves the matrix equation AX=B, where A is a symmetric coefficient matrix and B is a matrix of constant vectors. The determinant and inverse of A are also obtained.

ANL F105S, MATEQ, UNIQUE

This program, in subroutine (2) form, solves the matrix equation AX=B and obtains the generalized inverse of A, where A is any non-zero rectangular coefficient matrix and B is a matrix of constant vectors. In the case where this equation is unsolvable, a best solution in the least-squares sense is obtained.

ANL F251S, FRANCC

This program, in subroutine (3) form, finds all scalar solutions, λ_i (including proper multiplicity), to the matrix equation $Ax=\lambda x$, where A is an arbitrary complex square matrix.

ANL F455S, CROUTC

This program, in subroutine form, solves the matrix equation AX=B by the Crout method; here A is a complex square coefficient matrix and B is a matrix of constant vectors. The determinant of A is also obtained.

15S7066 ANGULAR DISTRIBUTION FOR FISSION FRAGMENTS

The program calculates angular distributions for fission fragments. The $W^J_{MK}(\theta)$ quantities calculated are automatically normalized by virtue of the recursive procedure used. These values are subsequently used in numerical integration steps of the program.

16S7076 FSCOPE — OSCILLOSCOPE AND LIGHT PEN DISPLAY

This SUBROUTINE subprogram, which is a FORTRAN version of the DIDJERIDOO function called SCOPER, provides for the display and analysis of one-parameter spectra by use of the DD16B oscilloscope and light pen.

17S7081 BINARY ("PSEUDO-BCD") TAPE ANALYSIS PROGRAM

Tape files, each consisting of from 1 to 16 physical records of 256 36-bit events, are analyzed and contents displayed in tabular and graphical form.

18S7082 BINARY DATA TAPE ANALYSIS

Binary data tapes of four or eight parameters per event and with 126 or 63 events per record are analyzed.

23S7098 ASI-TAPE READING PROGRAM

Subroutine RDMGTP is developed; it allows CDC 3600 reading of ASI 210 and 2100 tapes.

43S7158 TMC PAPER TAPE-TO-CARD CONVERSION

This program, written in OSAS assembly language for a CDC-160A, converts paper tape input to punched card output and produces a printed copy of the output data. Under selective jump switch option the punching may be bypassed and only a printed listing obtained.

45S8167 TRANSCRIBE SCIPP PAPER TAPE TO MAGNETIC TAPE

Paper tape data from a Victoreen model SCIPP 1600 multi-channel analyzer is converted from ASCII code to BCD equivalent and recorded on magnetic tape for subsequent processing by a CDC-3600 program.

46S8170 EQUILIBRIUM CONSTANTS RELATING SELENIUM SPECIES

This is an S/360 translation of the 704 program 1638/PHY 273.

49S8177 RECOMP PAPER TAPE TO BCD MAGNETIC TAPE CONVERSION

An edited magnetic tape is produced from an input magnetic tape onto which is copied one or more paper tapes.

50S8182 ARGONNE CODE CENTER TAPE COPY

This is a utility program designed for a 16K IBM 1401 system; it provides for copying of files from one magnetic tape to another. Tapes written in either BCD or binary mode are accepted. Information about the mode, number of records, lengtn of records, and number of files is printed during processing.

03T7006 LIBRARY DEVELOPMENT FOR IBM S/360 AND CONTROL DATA 3600

ANL E208S, ARBITRARY FUNCTIONAL FIT

This general program fits, in the least-squares sense, a set of observed values to an arbitrary function of up to 10 independent variables and up to 20 parameters.

ANL D253S, DDFSYS

This program is the driver to provide input/output and control for the double precision subroutine D2 ANL D252S DDFSUB, Integration of a System of First Order Ordinary Differential Equations.

ANL D252S, DDFSUB

This subroutine performs one double precision integration step for a system of first order ordinary differential equations using extrapolation by rational functions or by polynomial functions.

ANL D255 DFBND-DIFI

The subroutine DIFI uses an extrapolation by rational functions to perform one integration step for a system of (twenty or less) first order ordinary differential equations. The subroutine DFBND estimates the errors in the results of DIFI at the end of the integration step.

03T7006 LIBRARY DEVELOPMENT FOR IBM S/360 AND CONTROL DATA 3600 (Cont'd.)

ANL D256 DFBDRV

This program provides input/output and control for the two double precision 3600 FORTRAN routines DFBND-DIFI ANL D255, DIFI performs one integration step for a system of first order ordinary differential equations, and DFBND estimates the error in the results of DIFI.

ANL E206S, LSQPOL

This subroutine determines the coefficients of that polynomial of specified degree which best fits, in the least-square sense, a set of points.

ANL E209S, CALLSQ

This double precision program provides input/output and control for use with the double precision version of ANL E206S, LSQPOL to do a least-square polynomial fit.

ANL B456S, DCUBRT

This is a routine to evaluate the double precision cube root of a double precision floating point argument.

ANL D255S, DFBND-DIFI

The DFBND subroutine estimates the errors in the results of the subroutine DIFI; DIFI uses an extrapolation by rational functions to perform one integration step for a system of first order ordinary differential equations.

ANL D256S, DFBDRV

This program is a driver to provide input/output and control for the double precision subroutines DFBND and DIFI (ANL D255S).

ANL C372S, CHIPRB

This double precision function subprogram finds the probability that χ^2 for n degrees of freedom exceeds x, i.e., it calculates

$$\frac{1}{2^{n/2}\,\Gamma(n/2)}\int_x^\infty z^{n/2-1}\,e^{-z/2}\,dz \qquad (x \geq 0,\ n \geq 1).$$

03T7006 LIBRARY DEVELOPMENT FOR IBM S/360 AND CONTROL DATA 3600 (Cont'd.)

ANL C373S, DELIPK

This double precision function subprogram evaluates the complete elliptic integral $K(k^2)$ for $0 \leq k^2 < 1$.

ANL C374S, DELIPE

This double precision function subprogram evaluates the complete elliptic integral $E(k^2)$ for $0 \leq k^2 \leq 1$.

ANL C354S, ELLIPK

This function subprogram evaluates in single precision the complete elliptic integral $K(k^2)$, where $0 \leq k^2 < 1$, and

$$K(k^2) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - k^2 \sin^2\phi}}$$

ANL C355S, ELLIPE

This function subprogram evaluates in single precision the complete elliptic integral $E(k^2)$, where $0 \leq k^2 \leq 1$ and

$$E(k^2) = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2\phi}\, d\phi.$$

ANL C372, CHIPRB

This function subprogram finds the probability that χ^2 for n degrees of freedom exceeds x, i.e., it calculates

$$\frac{1}{2^{n/2}\,\Gamma(n/2)} \int_x^{\infty} z^{n/2-1}\, e^{-z/2}\, dz \qquad (x \geq 0,\ n \geq 1).$$

06T7010 TRAJECTORY CALCULATIONS FOR A MAGNETIC SPECTROMETER

The program calculates trajectories of charged particles through a variety of magnetic fields. The optional calculation of magnetic field values at specified coordinates and the calculation of optical coefficients are also available.

08T7019 CHEMICAL EQUATION TRANSLATOR

This program translates chemical equations representing chemical reactions and balance relations into FORTRAN source code for subroutines COEFF, MASBAL, and BLOCK DATA called by C146, Diffusion Kinetics IV.

17T7033 CONVERSION AND REDUCTION OF RIDL CHANNEL ANALYZER DATA

The preprocessor of Program P103 (subroutine PRESS) was modified to accept raw data in several different formats, to accept precomputed velocities, and to allow for fractional channel numbers.

23T7054 TABULATION OF TWO FUNCTIONS OCCURRING IN MESIC X-RAY CALCULATIONS

The functions $f_5(x,\beta)$ and $f_6(x,\beta)$ are tabulated in the interval $0 \leq x \leq x_{max}$ for various values of the parameter β. The functions are of the form

$$f(x,\beta) = \int_0^1 \phi(x,y,\beta)dy \ .$$

A numerical procedure is used to evaluate the integrals.

25T7059 THERMO-ELECTRIC POWER CALCULATIONS

The program reads thermocouple data or Germanium resistance thermometer data, obtains the corresponding temperatures, and then calculates and plots derivatives of a signal with respect to the temperature.

The program may also be used to calculate and plot derivatives of (x,y) data as input, or just to plot the input data.

26T7065 GERT, A FITTING PROGRAM FOR GERMANIUM RESISTANCE THERMOMETERS

This is a double precision routine to perform least-squares fits of orthogonal polynomials to resistance versus temperature calibration data for a germanium resistance thermometer.

29T7070 ESR LINE SHAPES IN MH_2AO_4 COMPOUNDS

Electron spin resonance line shapes in (MH_2AO_4)-type compounds are computed and plotted on the CALCOMP plotter.

39T7092 AN ALTERNATE PROCEDURE FOR CALCULATING ESR LINE SHAPES

Electron spin resonance line shapes are determined by evaluating a complex algebraic function and its first derivative over a specified range.

40T7097 VARIANCE ALGORITHM FOR MINIMIZATION

This is a new algorithm for minimizing differentiable functions.

50T7140 NEAREST NEIGHBOR INTERACTIONS IN CELL DYNAMICS

This model of cell division death and migration in organs requires determination of an eigenvalue and an eigenvector of a tri-diagonal matrix.

55T7151 DIAGONALIZATION OF COVARIANCE AND CORRELATION MATRICES

The eigenvalues and eigenvectors of covariance and correlation matrices either directly specified or formed from observational data are computed.

56T7160 GAUSSIAN UNFOLDING OF KX-RAY DISTRIBUTIONS

The program resolves a complex experimental pulse-height distribution by a least-squares technique into its individual components represented by Gaussian distributions. Given and built-in parameters determine the background, peak locations, widths, and the four relative peak heights for each element from atomic number 28 to 65. Peak heights are determined by fitting the function over a specified range of atomic numbers to observed values for up to 1024 channels.

62T8181 LEAST-SQUARES DETERMINATION OF SLATER PARAMETERS FROM OPTICAL SPECTRA

This program calculates values of Slater parameters giving a best fit with observed energy levels, where each element of the energy matrix is specified as a linear combination of the parameters. Successive least-squares iterations are made until the residual converges to a specified tolerance or diverges. The numerical matrix, eigenvalues, eigenvectors, (eigenvectors **2), and g-factors are calculated for each iteration.

The program is basically the same as C106 and C175 but with a provision for holding ratios of specified parameters constant, and for allowing for larger matrices and expanded input and output. This program may be used for cases with 30 parameters and 15 submatrices up to 100 x 100, with no more than 3600 off-diagonal coefficients in any one submatrix.

64T8190 NEAREST NEIGHBOR INTERACTIONS IN CELL DYNAMICS

This is an extension of 50T7140 wherein estimates of the smallest eigenvalue and its associated eigenvector are made from a specified formula and compared with those obtained from the eigenvalue/vector routine in 50T7140.

66T8195 UPDATING FORTRAN SOURCE CODE ON TAPE

A convenient method is provided to permit the modification of a FORTRAN program that is stored on tape. Only the changes to the program need be entered on cards.

70T8206 SPECIAL UNITS FOR COMPOSITE QUADRATIC FIELDS

This is a search for units of a biquadratic field which do not belong to its subfields, important in the determination of ideal structure.

B156 DETERMINATION OF RADIOISOTOPES BY LEAST-SQUARES RESOLUTION OF GAMMA SPECTRA (ORNL)

Program ALPHA M has been adapted for running on the CDC 3600. It is an improved version of program ALPHA, which was developed for the quantitative analysis of radioactive samples by the least-squares resolution of the gamma-ray spectra.

B186 A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

This program draws the crystal structure illustrations using the CALCOMP Magnetic Tape Plotting System #580. Ball-and-stick-type illustrations of a quality suitable for publication are produced with either spheres or thermal-motion probability ellipsoids on the atomic sites. The program can produce stereoscopic pairs of illustrations which aid in the visualization of complex packing arrangements of atoms and thermal motion patterns. Interatomic distances, bond angles, and principal axes of thermal motion are also calculated to aid the structural study.

This program is the same as one described in OR TEP: A FORTRAN THERMAL-ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS, a technical publication by Carroll K. Johnson, ORNL-3794, June 1965.

B212 LINEAR ENERGY TRANSFER ANALYSIS

This program represents an attempt to smooth raw data which originates in a multichannel analyzer. This data is smoothed in a way which appears to preserve legitimate peaks and valleys while keeping the sum of the raw data invariant. This is done by taking (or giving) a certain small fraction of the value associated with a given point and giving (or taking) this to an appropriate neighbor when it is obvious that this neighbor is not consistent with its neighborhood. The procedure uses a moving average of 3 neighbors and fourth finite differences. Our procedure differs from most smoothing techniques because we do not assume functional approximations and we do not attempt to adjust all points simultaneously. The smoothing procedure makes very small adjustments and is repeated many times.

B226 CALCULATION OF METAL-WATER REACTIONS DURING A LOSS OF REACTOR COOLANT ACCIDENT

This program determines the solutions to a system of partial differential equations which represent the extent of metal-water reactions during a loss-of-coolant accident.

B259 TEMPERATURE DECAY IN A CALORIMETER

The program B215 was modified to include the summing of chi-squared values over several sets of data.

B261 OVERLAY SYSTEM FOR THE B145, 14E, AND B114 PROGRAMS

This program provides a system for the use of the following crystallographic programs: B145, 14E, and B114. These programs are stored on a magnetic tape and the user may select any of the above programs individually or use them in a sequence. Sorting of reflection data for B114 is provided.

B262 PROMISE — REACTOR CORE DESIGN

This program searches for parameters which minimize the cost of a reactor core.

C123 SPECIAL THERMOMETER CALIBRATIONS DOWN TO .3°K (LOWCAL)

A calibration curve which is valid above .75°K is extended down to .3°K.

C125 FERMI-DIRAC FUNCTION

Function subprogram for the evaluation of the Fermi-Dirac functions $F_k(x)$ for $k = -1/2$, $1/2$, or $3/2$.

C146 DIFFUSION KINETICS IV

A system of partial differential equations representing diffusion and the kinetics of reaction of chemical species is solved to give the concentrations of the various species as a function of space and time. Space integrals which give the total number of molecules of each species in the solution are calculated as a function of time. Calculations may be done for either spherical or cylindrical symmetry. The system is solved using a modified Crank-Nicolson method that gives stable implicit solutions over relatively large time steps.

C155 PROTON MAGNETIC RESONANCE LINESHAPE

The program calculates and plots derivatives of Gaussians.

C181 COMPUTATION OF SLATER-PARAMETER COEFFICIENTS, ENERGY LEVELS, AND ATOMIC SPECTRA, RCG - MOD1

For an arbitrary electron configuration analytical expressions are written for the energy-matrix coefficients of the electrostatic-interaction parameters and of the spin-orbit parameters. The program calculates decimal values of these coefficients for any configuration with less than four open shells starting from a table of the terms, parents, and coefficients of fractional parentage for each open shell. Given also a set of values of the parameters, the program evaluates and diagonalizes the energy matrices to obtain the eigenvalues and eigenvectors of the states belonging to this configuration.

The program is a modification of a program written by Robert D. Cowan of Los Alamos Scientific Laboratory.

C186 PARTICLE COUNTS AT SURFACE OF FLUIDIZED BED

This program reads the magnetic tape prepared by the CHLOE Liberator System, and obtains a time series given by the frame-by-frame count of tracer particles. From the above time series, the program then calculates the autocovariances of "sample moments" and corrects the input data by assuming a theoretical distribution in the changes in the counts and discarding the improbable events.

Then, if needed, the program fits the observed and corrected sample moments to the best theoretical autocovariances and thus arrives at a "best" fitted residence time density for the particles in the time series. An option to read the data from cards is provided.

H131 POLLY I — CALIBRATE MEASURING

A method is provided for calibrating of the POLLY film scanner when viewing bubble chamber pictures. The coordinates determined are collected and recorded on magnetic tape for subsequent processing.

P157 ASI-210 EXTERNAL MEMORY SYSTEM PROGRAMS

Three separate programs are included in this project, which is in support of the 96K external core memory attached to the Physics Division ASI-210 computer.

1. (P157A) This is an engineer's diagnostic program for checking the proper functioning of the external memory.
2. (P157B) This is a subroutine for performing I/O functions between the external memory and the computer's main memory.
3. (P157C) This is a link calling subroutine utilizing the external memory in an overlay system.

R147 PPHX1 — COUNTER-CURRENT FLOW PARALLEL PIPE HEAT EXCHANGER

This program solves an infinite set of linear integral equations.

R154 BIRDIE — ROCKET CYCLE ANALYSIS

This is a nuclear rocket cycle analysis program.

R2000 DPLOAD, AN ARC DATAPOOL LOADER

This is a module for ARC, the Argonne Reactor Computation system.

R49010 NUE001, OUTMAN, AN ARC MODULE FOR NEUTRONICS OUTPUT MANIPULATION

This is a module for ARC, the Argonne Reactor Computation system.

Key to program labels:

E Experimental Science
S Engineering and Applied Systems
T Theoretical Physics and Chemistry
R Reactor Theory and Development
P Physics Applications
C Chemical Applications
B Biological and Metallurgical Applications
H High Energy Physics Applications
I Information Processing Applications

Listed below by title are those programs still in progress at the end of the report year:

001E6001	ELECTRON MICROPROBE DATA ANALYSIS
003E6009	CONSULTATION ON VARIOUS CRYSTALLOGRAPHIC PROGRAMS
004E6010	CONSULTATION ON VARIOUS CRYSTALLOGRAPHIC PROGRAMS
13E7042	RESISTIVITY OF THIN FILMS
15E7051	METAL-WATER REACTIONS DURING ACCIDENT
18E7060	ANALYSIS OF EBR2 FUEL PIN SWELLING
20E7063	HEATING RATES IN A^2R^2 SUPPORT STRUCTURES
21E7064	CALCULATION OF STORED ENERGY IN RADIATED MATERIALS
22E7067	APPLIED PROGRAMMING EFFORT
23E7074	HFIR IBT-SPOT CODE
26E7085	CALCULATION OF DAMAGE RATE DERIVATIVES
27E7090	DIRECT METHOD USING TANGENT FORMULA
28E7091	ANALYSIS OF STRESS-STRAIN DATA
29E7096	TEMPERATURE DEPENDENCE OF THIN FILM RESISTIVITY
30E7095	SIGN DETERMINATION FOR CENTROSYMMETRIC CRYSTALS
34E7113	REPORT GENERATION
35E7117	CALCULATION OF DIFFUSION RATES IN ALUMINUM ALLOYS
37E7119	A FORTRAN PROGRAM FOR CALCULATING SINGLE CRYSTAL ABSORPTION CORRECTIONS
40E7146	STATISTICAL PROGRAM LIBRARY
41E7147	CDC TEST PROGRAM
42E7149	CHECK OF A^2R^2 STRESS-STRAIN CALCULATIONS
44E7154	COMPACTION PROFILE MEASUREMENT
45E7155	MONTE CARLO EVALUATION
46E7156	CRYSTAL CONDUCTIVITY FIT
47E7159	CALCULATION OF RESISTIVITY

48E7161	COUNT ACCUMULATION
49E8172	ION TRAJECTORIES IN AN ELECTROSTATIC FIELD
50E8174	FUEL USE ANALYSIS
51E8175	AUTOFLOW PREPARATION
52E8185	DETERMINATION OF SURFACE TENSIONS FROM PHOTOGRAPHED MENISCI
54E8192	AARR PROCUREMENT SCHEDULE
56E8197	CYGRO — FUEL ROD STRESS EVALUATION
59E8201	GEMANL — 360 VERSION OF PROGRAM GEM
60E8202	CROSS-SECTION COMPUTATION
62E8207	STATISTICAL ANALYSIS OF DEFECTS IN NONSTOICHIOMETRIC METAL OXIDES
01R6005	TRANSPORT THEORY SEMINARS
02R7001	RE138 AND RE171 FOR THE 3600
04R7010	PETER
05R7011	HOMOGENIZATION INPUT
06R7012	HOMOGENIZATION
08R7029	STOCHASTIC PROBLEMS IN TRANSPORT THEORY
11R7068	GROWTH OF TWO COMPETING POPULATIONS
15R7110	CHICAGO AIR POLLUTION SYSTEM MODEL
16R7116	SLIGEN — SOLUTION OF A STURM-LIOUVILLE SYSTEM
17R7148	ACCIDENTAL LOSS OF COOLANT STUDY: FLASH II
18R7153	3600 CANDID CORRECTION
19R8176	NEUTRON FLUX METHOD OF BOILING DETECTION
01S6001	PROGRAMMING AND COMPUTING FOR THE FAST NEUTRON HODOSCOPE
03S7002	ANALYSIS OF BINARY NUCLEAR FISSION DATA TAPES
08S7013	LINKAGE FROM PL/1 TO FORTRAN AND VICE VERSA
14S7061	INTRINSIC MULTIPROCESSOR SIMULATION
19S7083	LIBRARY SERVICES SUBROUTINE PACKAGE
20S7084	JOURNAL RENEWAL SYSTEM

22S7089	PRELIMINARY ANALYSIS OF Ge(Li) DETECTOR SYSTEM (LIVERMORE)
24S7112	ENERGY DISTRIBUTION FOR GAMMA RAYS IN WATER
25S7121	SELECTOR — SELECTOR FILE PREPARATION FOR BOOK ACQUISITION
25S7122	STACK — PREPROCESSOR FOR SELECTOR
26S7123	DISTRIB: A PROGRAM TO PRINT SELECTOR LISTS FOR BRANCH LIBRARIES
27S7124	VALIDATE: A PROGRAM TO PREPARE ENTRIES TO THE "IN PROCESS" FILE
28S7125	LIBAQ: A LIBRARY BOOK AQUISITIONS SYSTEM
29S7126	LANGUAGE DEVELOPMENT FOR EXPERIMENTAL CONTROL
30S7127	INFORMATION RETRIEVAL USING CDC 3600
31S7128	DAVIS FUND USAGE REPORT
32S7129	INFORMATION RETRIEVAL ON SYSTEM/360
33S7130	SPP MAINTENANCE
34S7131	CASE STUDY FOR 3600 CDC KWIC
35S7132	DSP FOR RADS
36S7133	3600 JOB LIBRARY MAINTENANCE
37S7134	SYSTEM/360 ODDJOB MAINTENANCE
38S7137	3600 TO 360 TRANSDECK PROGRAM
39S7145	X-RAY DIFFRACTOMETER PROGRAM
40S7150	ARGOS — DMP AND JCL COMPILER
42S8157	BOOLEAN ALGEBRA REDUCTION
44S8165	RESPONSE PARAMETERS FOR NEUTRONS INCIDENT ON A Ge DETECTOR
47S8171	X-RAY DIFFRACTION
48S8173	RESPONSE PARAMETERS FOR X-RAYS IN GERMANIUM
51S8183	ARCADE VARIABLE BACKGROUND SCAN
52S8186	ANL TECHNICAL PUBLICATIONS ANNUAL REPORT
53S8188	PAPER TAPE TO MAGNETIC TAPE TRANSCRIPTION
54S8189	META-SUMX
55S8193	TAPEOUT, MAGNETIC TAPE TO PRINTER OR PUNCH

56S8204	3600 SCOPE SYSTEM GENERATION
57S8210	RADS STATION DEVELOPMENT
04T7008	ARGONNE CODE CENTER
05T6003	COMBINED CONDUCTION-RADIATION PROBLEM, INCLUDING TRANSIENTS
09T7022	BUBBLE CHAMBER FLOW DYNAMICS
11T7024	CALCULATION OF CUBIC HARMONICS
13T7026	CONFIGURATION INTERACTIONS — FANO
16T7032	CALCULATION OF ELECTRONIC TRANSITION PROBABILITIES
18T7036	DETERMINATION OF FERMI SURFACE FROM DeHAAS van ALPHEN MEASUREMENTS
19T7038	THERMOCOUPLE CALIBRATION PROGRAM
20T7049	POLYNOMIAL FACTORIZATION
21T7050	PROGRAMMING CONSULTANT SERVICES
22T7052	DIFFERENTIAL EQUATION SOLVER
24T7058	FISSION FRAGMENT MATRIX ANALYSIS
27T7068	MODEL OF BIOLOGICAL SYSTEM
32T7077	REDUCTION OF GROUP REPRESENTATIONS
33T7078	STRESS, STRAIN, AND CREEP COMPUTATIONS
35T7086	MONTE CARLO CALCULATIONS
36T7087	FOURIER TRANSFORMS OF TIME-LIMITED SIGNALS
37T7088	PROGRAM DEVELOPMENT AND DEBUGGING
38T7089	PRELIMINARY ANALYSIS OF Ge(Li) DETECTOR SYSTEM (LIVERMORE)
41T7100	DETERMINATION OF HYPERFINE COUPLING TENSORS
42T7101	BIM 130
43T7105	EDUCATIONAL AND ADVISORY SERVICES
44T7107	ALL ROOTS OF POLYNOMIAL EQUATIONS WITH REAL COEFFICIENTS
45T7108	THTB (GE) — THREE-DIMENSIONAL TRANSIENT HEAT TRANSFER
46T7115	SUPERCONDUCTING LENS OPTIMIZATION
47T7120	CURVE-FITTING FUNCTION SPECIFICATION

48T7135	TEMPERATURE DISTRIBUTION IN A CYLINDRICAL FUEL-ROD ASSEMBLY
49T7136	CALCULATION OF CUBIC HARMONICS
51T7141	ABEL INVERSION COMPUTATION
52T7142	LINDHARD'S CROSS SECTION
53T7143	INTEGRAL EQUATIONS DETERMINING ION RANGE AND DAMAGE
54T7138	TEMPERATURE DISTRIBUTION IN A CYLINDRICAL FUEL-ROD ASSEMBLY
57T8162	INSTRUCTION IN USE OF FORTRAN
58T8164	TEMPERATURE DISTRIBUTION IN A CYLINDRICAL FUEL-ROD ASSEMBLY
59T8166	HYDROLYSIS AND FILTRATION BY LEAST SQUARES FIT
60T8168	COMPUTATION OF SLATER-PARAMETER COEFFICIENTS, ENERGY LEVELS, AND ATOMIC SPECTRA
61T8169	THFNS — FIT OF THERMODYNAMIC PROPERTIES
63T8184	ANALYSIS OF EBR2 FUEL PIN SWELLING
65T8191	TRANSLATOR: BURROUGHS ALGOL TO 3600 ALGOL AND 360 ALGOL
67T9196	SPECTRUM GENERATION AND FITTING ROUTINE
68T8198	CREEP STRAIN IN EBR-II MARK II FUEL ELEMENT CLADDING
69T8203	MÖSSBAUER SPECTROSCOPY
71T8208	STATISTICAL ANALYSIS
72T8209	MAGNETIC MOMENT EVALUATION
73T8213	FORTRAN JULIE — CALCULATION OF DIFFERENTIAL CROSS SECTIONS
B141	DESIGN OF 750-KEV ACCELERATING COLUMN
B193	ELECTRODE POTENTIAL VS. POLARIZING CURRENT
B195	SIMULATION OF LABELED MITOSIS CURVES
B196	BAND STRUCTURE CALCULATION
B199	BIG BUBBLE CHAMBER CONVECTIVE FLOW
B203	CRYSTALLOGRAPHIC CONTOUR MAPS
B204	A FIT OF CRYSTAL FIELD EQUATIONS TO MAGNETIC SUSCEPTIBILITY DATA
B205	VAPOR PRESSURE CALCULATIONS

B206	STUDY OF AUTOCORRELATION OF A STATIONARY BIRTH AND DEATH PROCESS
B210	LEAST-SQUARE REFINEMENT PROGRAM
B211	DETERMINATION OF CRYSTAL STRUCTURE
B213	CRYSTALLOGRAPHIC PROGRAMS FOR THE 1130
B216	IRREVERSIBLE TRANSFER IN A BIMETALLIC CELL
B221	CALCULATION OF EXPERIMENTAL CAPTURE CROSS SECTIONS
B222	DETERMINATION OF ISOTOPIC RATIOS WITH MULTICHANNEL ANALYSES
B227	ALGEBRAIC COMPUTATIONS IN COGENT
B230	SINGLE-CRYSTAL NEUTRON DIFFRACTION DATA PROCESSING
B232	PARTICLE MOVEMENT IN A SWARM OF RISING BUBBLES
B235	CORROSION APPROXIMATION
B236	FIT OF RESISTIVITY VS. RADIATION DOSE
B244	ANALYSIS OF STRESS AND STRAIN DATA
B247	A FIT TO REDUCE CROSS SECTIONS
B250	WIENER INTEGRALS AND TAXONOMY
B260	NEUTRON DIFFRACTION DATA REDUCTION AND EXTINCTION CORRECTION
C144	WIDTH CALCULATIONS IN METALS
C147	EXPERIMENTAL DATA ANALYSIS — RESISTIVITY VERSUS TEMPERATURE
C152	DECAY OF TWO INTERACTING SPECIES
C157	INTERTHERMOMETER COMPARISON
C161	RESOLUTION CORRECTION
C164	DETERMINATION OF RATE CONSTANTS FOR CHEMICAL REACTIONS
C170	FISSION FRAGMENT CORRELATIONS
C171	FREQUENCY FUNCTIONS OF A LIQUID
C172	ASI MULTIPARAMETER ANALYSIS
C179	SPIN LATTICE RELAXATION IN MÖSSBAUER SPECTRA
C187	CHECKING EQUATIONS FOR ODD U^K MATRIX ELEMENTS
C188	FITTING NEUTRON DIFFRACTION PATTERN

C190	I/O SUBROUTINES FOR SYSTEM 360
C192	CURVE FITTING FUNCTION SPECIFICATION
C194	MEASUREMENTS OF FAST REACTIONS IN RADIATION CHEMISTRY
C196	CALCULATION OF IODINE INHALATION RADIATION DOSES — AD HOC PANEL ON AARR SAFETY EVALUATION
C198	CALCULATION OF RADIATION DOSE RATIOS — AD HOC PANEL ON AARR SAFETY EVALUATION
C200	CONFIGURATION INTERACTIONS WITH f^n CORE
H122	MAP — SPATIAL RECONSTRUCTION OF WIDE GAP SPARK CHAMBER TRACKS
H123	PRINTAP2
H124	INTERMEDIATE BOSON CROSS-SECTION CALCULATION
H126	GENRAT — SIMULATION OF BUBBLE CHAMBER EVENTS
H127	MAESTRO — A PROGRAM FOR THE REAL TIME GENERATION OF MUSICAL SOUNDS
H128	AUTOMATIC PROCESSING OF LAMBDA-BETA DECAY EXPERIMENT
H129	AUTOMATIC PROCESSING OF SIGMA MAGNETIC MOMENT EXPERIMENT
H130	GRAPHICAL MAN-MACHINE INTERFACING
I100	DATA ACQUISITION AND/OR TIME-SHARING VIA REMOTE CONSOLE
I101	MONTE CARLO MODEL FOR 3600 OPERATIONS
I102	PERT STUDY FOR SYSTEM/360 ACQUISITION
I104	TOPOLOGICAL PROPERTIES OF TWO-DIMENSIONAL SELF-RESTRICTING MAZES
I106	SELECTIVE DISSEMINATION OF INFORMATION UTILITY ROUTINE
I110	FINGERPRINT CLASSIFICATION AND IDENTIFICATION
I113	SDI MATCHING PROGRAM
I116	TPD BUDGET AND TYPE COUNTING ROUTINE
I117	ORIENTATION AND ANGLE SETTING GENERATION
I118	COMPLEX SPECTRA ANALYSIS IN HUMANS
I119	LOW ENERGY ELECTRON RESPONSE SPECTRA IN SILICON
I120	PATTERN RECOGNITION TEST
P140	CALCULATIONS OF SPIN-SPIN RELAXATION IN $FE(NH_4)\ (SO_4)$

P144	MÖSSBAUER OPTIMIZATION
P147	CHOPPER TRANSMISSION ANALYSIS
P153	ABACUS
P154	FOUR-PARAMETER ANALYZER ANALYSIS
P156	PHYLIS LIBRARY TAPE SYSTEM
P160	ASSEMBLER FOR THE IBM 1130
P167	FIT HAMILTONIAN TO SPECTRA
P180	ND 160 COMMUNICATION PROGRAMS VIA B05
R149	TRAFICORPORATION
R150	SYSTEMS EVALUATION
R151	UO_2 PHONON DISTRIBUTION
R152	CANDID
R155	PRELIMINARY DESIGN OF AN INDUCTION MHD GENERATOR
R157	DOPPLER BROADENED CROSS SECTIONS
R160	LIQUID FILM GENERATOR OPEN AND CLOSED CIRCUIT ANALYSIS
R161	DEFLECTION AND STRESS ANALYSIS FOR THIN PLATES AND TUBES
R163	CANDID1D
R164	MHD CYCLE EFFICIENCY ANALYSIS
R165	MISCELLANEOUS PROGRAMS (AMD PROGRAM LIBRARY)
R166	TRANSCENDENTAL BESSEL EQUATION ROOTS
R167	TRANSPORT DELAY SUBROUTINE
R168	COOLANT EXPULSION STUDIES — DATA REDUCTION
R169	SATURATED — COUNT RATE CALCULATION FOR ACTIVATED LIQUIDS
R171	MISCELLANEOUS REACTOR CALCULATIONS
R172	NUCLEAR SAFETY — ACCIDENT ANALYSIS
R173	MATHEMATICAL RESEARCH AND PROGRAM DEVELOPMENT (REACTOR DESIGN)
R174	PRELER III — PRESSURE AND LEAKAGE RATE TEST FOR EBWR
R175	TECHNICAL PROGRAM COMMITTEE SERVICE

DIGITAL COMPUTER OPERATIONS

During the report period most of the computational assistance for Argonne scientists was provided by the IBM System/360 Models 75 and 50 and the CONTROL DATA 3600.

IBM S/360

The IBM System 360/50/75, operated under the Attached Support Processor (ASP) system, was processing more than 7500 jobs per month by the end of the reporting period. Highest priority was given to jobs of 1 minute or less duration, with subsequent priority limits of 2 minutes, 3 minutes, 4 minutes, 5 to 9 minutes, 10 to 14 minutes, 15 to 29 minutes, 30 to 59 minutes, and 60 minutes and over.

A "multiple console" concept of operations was used; it usually included three input and recording devices and one logging device. At various times these included one or more of the following: IBM 1052, IBM 1053, IBM 2741, Teletype 33.

During the year film plotting using the 2280 Film Recorder was performed, and batching of output in the nonprocess mode was utilized.

Performance reliability for the System 360 varied: following an initial unstable "shake down" period of several months, there was a period of relative reliability. In May and June, however, hardware difficulties returned and reliability declined. The cumulative statistics for the year ending June 30, 1968 show that 19.2 percent of the available system hours were not useful; these were about equally divided among uncharged computer reruns (5.6%), scheduled maintenance (5.1%), unscheduled maintenance (5.3%), and installation of engineering changes (3.2%). During May and June hardware system failures averaged seven or eight per day, and varied in their effect from the need merely to reload the system program to the loss of all input and output queues; an average of two to three hours of machine time were lost per day to reruns and unscheduled maintenance.

CONTROL DATA 3600

The CONTROL DATA 3600 was operated around the clock during the year except for several holiday periods totalling about four days. This computer continued to operate in a reliable manner, with an availability record of over 90 percent and an unscheduled maintenance record of only .8 percent for the year. Most of the unscheduled maintenance involved the DD80 film output device and the CDC 828 disk file. The smaller CONTROL DATA 160-A's were equally reliable. Single-shift maintenance for five days per week was purchased from Control Data for the 3600 and four 160-A computers.

During prime time, computations of less than five minutes' total duration were expedited and when no jobs of this category were available, jobs of less than ten minutes were run. Longer jobs and attended runs were completed as time permitted. During normal weekdays, 200 to 300 jobs were run on the prime shift. A feature of the weekday early evening operation was the provision of several expedited turnarounds, thus materially helping programmers on a "crash" schedule. An average of 150 jobs of varying lengths were completed during the remaining evening and early morning hours. Approximately 150 jobs of various lengths were run on weekends, including those run during the expedited schedule hours of 2 to 5 PM.

IBM 1401

In February 1968 the 1401 that had been operating since 1961 in the Applied Mathematics Division was transferred to the Physics Division. Simultaneously, the 1401 which had been in the Accounting Department since 1963 was transferred to Applied Mathematics. Since this exchange, users have been provided with 7-channel, 800 BPI tape density service as well as the large capacity memory (16K) of this 1401.

The machine transferred to Applied Mathematics has been reliable after an initial unstable period. Maintenance is provided by IBM under a single-shift, five-days-per-week contract.

REMOTE STATIONS

Microwave communication is maintained between a remote station located in the High Energy Physics (HEP) and Applied Mathematics (AMD) Buildings.

Input jobs to be run on the 3600 are submitted by HEP users to the CONTROL DATA 160-A operator in the HEP Building; he prepares an input tape. A microwave telephone hookup is used to establish feasibility of transmission, and the operation is initiated when both stations are ready. Each station is capable either of receiving or of transmitting. Normal practice is to transmit 3600 input tapes from the HEP Building to the AMD Building and to send 3600 output tapes from AMD to HEP.

The transmission schedule currently is on an informal basis. At the discretion of the operator in the HEP Building, input tapes are sent whenever a sufficient number of jobs have been collected or if the elapsed time is about two hours. This has insured the HEP users between two and three turnarounds per day. Transmission reliability has been high and the duration of transmission is relatively short, so that a retransmission is very practical in the event of error.

The 160-A computer in HEP is engaged in various routine data editing and data transfer jobs, in addition to its transmission assignments.

The 160-A computer in the Reactor Divisions Building is active with programs for those who wish to write and perform their own computations. A considerable amount of data transfer from paper tape to other forms is undertaken; there is much plotting from data using a Calcomp incremental plotter.

GENERAL

Cathode ray tube (CRT) output on the 3600 and System 360 is being emphasized by the development of film using an Eastman Kodak Recordak, modified to accept the take-up reel of the CRT film camera and capable of developing 5 feet of film per minute. Volume averages 1500 pictures per day, representing output from 5 percent to 8 percent of all jobs run.

Tape storage charges of $1 per month for archival tapes (unused for 60 days) were started in November 1967. The charge is intended to encourage the release of reels of low utility. Initially, hundreds of reels were released. In November, 3822 reels were subject to the charge; by the end of June there were more than 5700 archival reels.

Tape reel testing and retesting continues to be necessary, and many man hours a week are required for that operation.

OPERATIONS EXPERIENCE DURING THE PERIOD JULY 1, 1967 - JUNE 30, 1968

	Hours						
	Charged & Sustaining	Setup	Uncharged	Maintenance Sched.	Maintenance Unsched.	Unused	Engineering
CDC 3600	7389.3	138.4	192.8	524.9	66.2	392.8	74.8
IBM System 360	4203.9	22.2	490.3	451.2	468.1	2865.8	280.5
CDC 160A Off-line	8130.0	0	0	104.0	26.0	520.0	0
CDC 160A HEP	2373.8	0	0	92.4	33.9	6283.7	0
CDC 160A Reactor	2677.6	0	0	93.81	48.53	5960.0	0
IBM 1401	3836.47	0	14.84	46.31	102.02	4746.48	33.41
CHLOE	1247.8	0	0	105.0	140.5	7197.3	92.9
7094 (purchased time from U. of Chicago)	121.76						
ANALOG	775.0						

1a. Charged — All computing and processing of data including the development of computer programs, except as noted below. A transfer of funds is involved for all time in this category. (Research time used by the Applied Mathematics Division staff is included here.)

1b. Sustaining — Use of authorized AMD personnel for the following purposes: developing and testing of programming systems supporting the use of the computer, demonstrations, training, and reliability testing of hardware and software, except as noted below.

2. Setup — Time consumed in setting up tapes and equipment for a "batch" of jobs processed by the monitor system.

3. Uncharged — Computer use for reruns attributable to the malfunction of the computer or peripheral equipment, supplied or AMD-supported programming systems, or to AMD clerical or operating errors.

4. Scheduled Maintenance — Time consumed for scheduled preventive maintenance by customer engineers.

5. Unscheduled Maintenance — Time elapsed between the request for, and the completion of, corrective action required by equipment malfunction.

6. Unused — Computer time not otherwise accounted for.

7. Engineering — Time consumed for Engineering changes, new attachments, and acceptance testing, by either ANL or computer manufacturer's personnel.

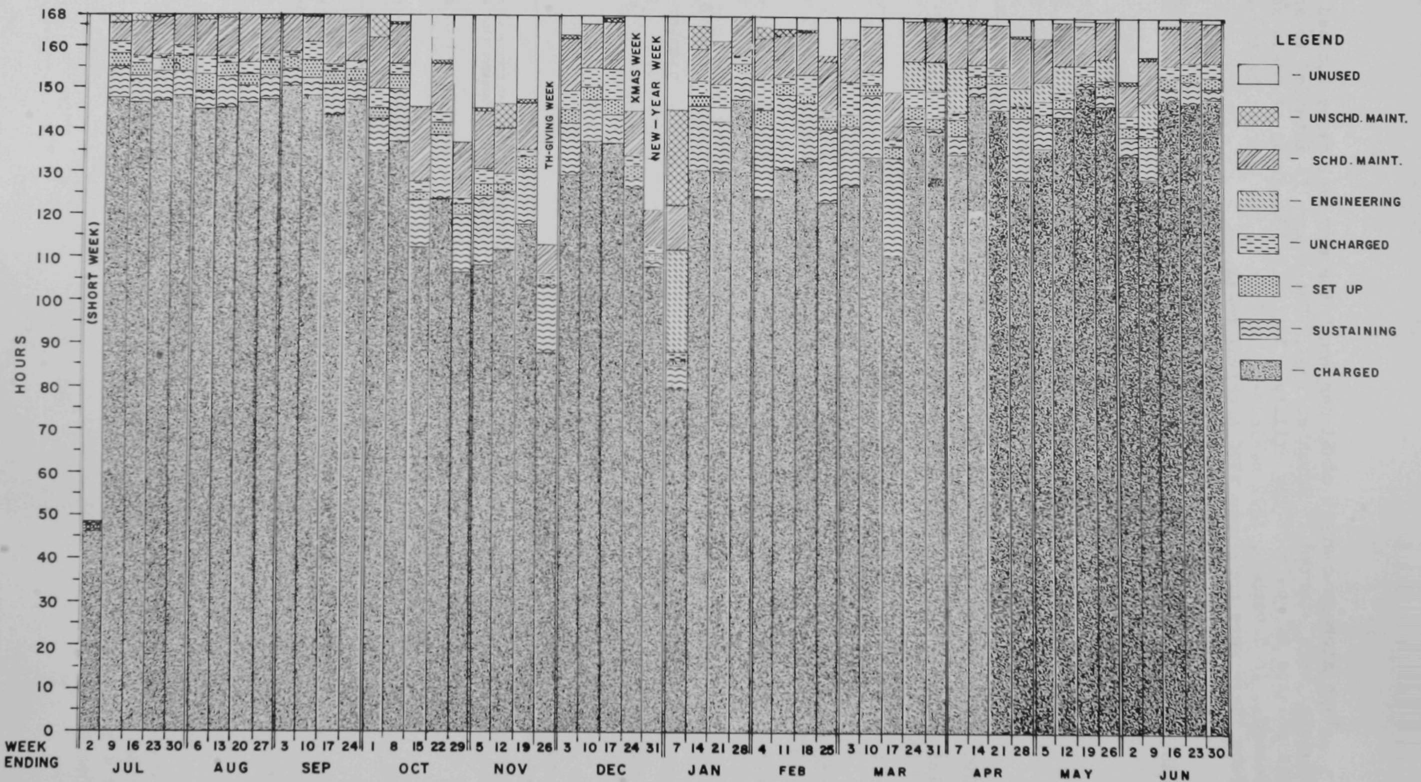
Other equipment, for which formal statistics are not maintained:

Calcomp Plotters — Operated 12 to 24 hours per day, 7 days per week.

CDC 160-A (Satellited to 3600) — Used approximately same hours as the 3600.

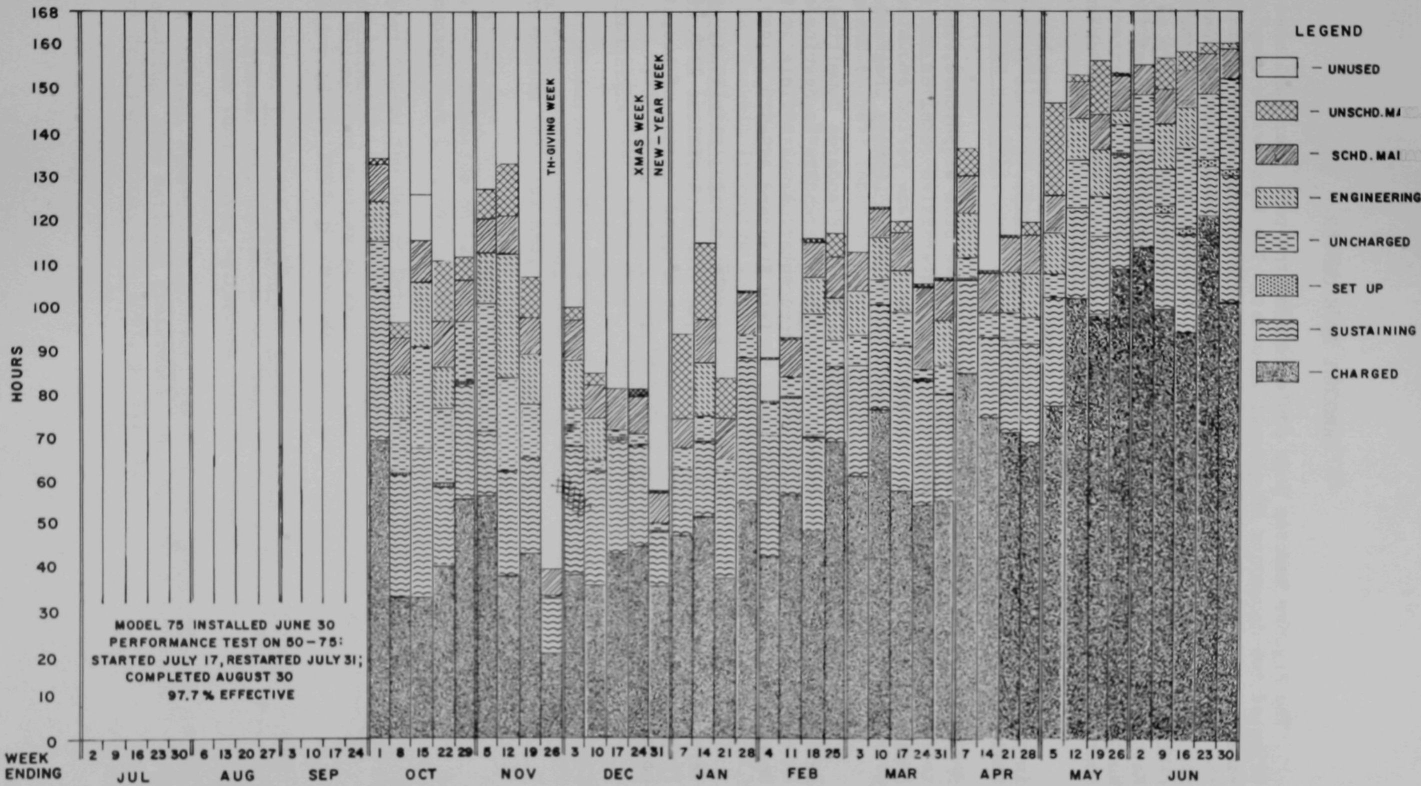
3600 COMPUTER USE

JULY 1967 THRU JUNE 1968



IBM MODEL 50/75 COMPUTER USE

JULY 1967 THRU JUNE 1968



ARGONNE CODE CENTER

The Argonne Reactor Code Center during the past year published and distributed two documents of general interest. The first was a completely revised collection of program abstracts prepared by the Center staff (ANL-7411); the second was the initial compilation of benchmark problems prepared by the ANS Mathematics and Computation Division's Benchmark Problem Committee (ANL-7416). Both reports were distributed to interested members of the Mathematics and Computation and the Reactor Physics Divisions of the American Nuclear Society by the Society, to Center Installation Representatives by the Center, and to TID recipients through regular AEC distribution channels.

In addition, regular reports of Code Center activity have been included in the monthly ANL Reactor Development Progress Reports since February of this year.

During the year 848 program packages have been dispatched, including 717 to requestors within the United States. Universities received 153 of these packages. Additions to the library during this same period amounted to 105 programs; 26 of these were ENEA Computer Programme Library programs.

Cooperative work continued with the ANS-10 Standards Committee, where a set of programming guidelines to facilitate interchange is nearing completion. An earlier effort on computer program documentation was officially released in December, 1967, as American Nuclear Society Standard ANS-STD.2-1967.

Work was initiated on the ACCESS program storage, retrieval, and distribution system for the IBM-360 in conjunction with similar ENEA Computer Programme Library objectives but had to be dropped because of budget considerations.

PUBLICATIONS AND PAPERS

Publications

1) W. E. Smith, Electric and Magnetic Energy Storage in Passive Nonreciprocal Networks, Electronics Letters (U.K.) 3(8),389-391 (August 1967).

2) W. J. Cody, Another Aspect of Economical Polynomials, Comm. ACM 10(9),531 (September 1967) (Letter to the Editor).

3) W. Gautschi, Numerical Quadrature in the Presence of a Singularity, SIAM Journal on Numerical Analysis 4(3), 357-362 (September 1967).

4) Kenneth Hillstrom, Remark on Correction to Certification of Algorithm 279 (D1), Comm. ACM 10, 666 (October 1967).

5) L. Wos, G. Robinson, D. Carson, L. Shalla, The Concept of Demodulation in Theorem Proving, Jour. ACM 14(4), 698-709 (October 1967).

6) J. M. Cook, Branching Processes and Reactor Theory, Trans. ANS 10(2), 521 (November 1967) (Abstract).

7) W. E. Smith, Energy Density of Acoustic Waves in a Plasma, Proceedings Letters, Proceedings of the IEEE 55(11), 2051-2052 (November 1967).

8) W. Roy Wessel, Iterative Quadratically Convergent Algorithm for Solving the General Hartree-Fock-Roothaan Equations, Jour. Chem. Phys 47(9), 3253-3256 (November 1, 1967).

9) J. Van Ryzin, A Stochastic a posteriori Updating Algorithm for Pattern Recognition, Jour. Math. Anal. & Appl. 20(2), 359-379 (November 1967).

10) M. D. MacLaren and M. E. Mahowald[1], A Machine Calculation of a Spectral Sequence, in "Mathematical Aspects of Computer Science" (Symposium Applied Mathematics Vol. 19) AMS, 117-124 (1967).

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[3] High Energy Physics Division
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Applied Mathematics Division Technical Memoranda

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[1] High Energy Physics Division.

Papers Presented at Meetings

1) A Computer-Controlled Electron Microscope System, by J. W. Butler. MICRO-67 Conference, Cambridge, England, August 21-25, 1967.

2) Optics of Axially Symmetric Electron Lenses, by J. W. Butler. MICRO-67 Conference, Cambridge, England, August 21-25, 1967.

3) Argonne Computer Aided Diffraction Equipment, by M. H. Mueller[1], L. Heaton[1], R. A. Aschenbrenner, and L. W. Amiot. American Crystallographic Association Summer Meeting, University of Minnesota, Minneapolis, Minnesota, August 20-25, 1967 (abstracted in program of meeting).

4) Microprogramming Revisited, by M. Flynn and M. D. MacLaren. ACM Conference, Washington, D.C., August 29-31, 1967.

5) Numerical Algorithms Based on the Theory of Complex Variables, by J. N. Lyness. ACM 20th Anniversary Meeting, August 29-31, 1967, Washington, D.C.

6) Computer Analysis of Autoradiographs, by J. W. Butler. EURATOM C.C.R., Ispra, Italy, September 8, 1967.

7) Performance Tests of a Computer System for the Analysis of Chromosome Images, by J. W. Butler. Cytogenetics Group Meeting, Michael Reese Hospital and Medical Center, Chicago, Ill., October 12, 1967.

8) A Computer-Controlled Electron Microscope System, by J. W. Butler. AEC Computer Information Meeting, Brookhaven National Laboratory, November 1-2, 1967.

9) Branching Processes and Reactor Theory, by Joseph M. Cook. ANS 1967 Winter Meeting, November 8, 1967.

10) High Frequency Magnetic and Electric Polarizabilities of a Plasma Sphere, by W. E. Smith. American Physical Society, Plasma Physics Division, Austin, Texas, November 11, 1967.

11) Quasisimple Representations and Induced Representations of Lie Groups, by E. Thieleker. American Mathematical Society Meeting, San Francisco, California, January 23-27, 1968.

12) POLLY, An Automated Bubble Chamber Film Measuring System, by Donald Hodges. AEC Advisory Committee Meeting, January 24-25, 1968.

13) Operations and the Logic of Quantum Mechanics, by James C. T. Pool. Annual Meeting of the American Physical Society, Chicago, Ill., January 29-February 1, 1968.

14) Program Documentation, by Clifford G. Levee, Discussion Leader. Data Processing Management, University of Wisconsin, Madison, Wisconsin, March 26-28, 1968.

15) Maximal Model Theory, by L. Wos and G. Robinson. Completeness of Paramodulation, by G. Robinson and L. Wos. Abstracts by title, Association for Symbolic Logic, San Francisco, California, March 1968.

16) Machine Extraction of Ridge Endings from a Noisy Fingerprint, by C. B. Shelman. Second National Symposium on Law Enforcement, Science, and Technology, sponsored by the Department of Justice, Chicago, Ill., April 16-18, 1968.

17) Systems Design for a Computer-Controlled Electron Microscope, by J. W. Butler. INTER/MICRO-68 Conference, June 10-14, 1968, Chicago, Ill.

18) An Iterative Method for Solving Multi-Variable Extremum Problems with Constraints, by Roy Wessel. SIAM 1968 National Meeting, Toronto, Ont., Canada, June 13-14, 1968.

19) The Function of a Technology: Some Comments on LSI, by Michael J. Flynn. IEEE Second Annual Computer Conference, Los Angeles, California, June 24-26, 1968.

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[1] Metallurgy Division
[2] Physics Division

University and Symposium Presentations

1) Numerical Algorithms Based on the Theory of Complex Variable, by J. Lyness. Computer Science Department Seminar, Purdue University, Lafayette, Indiana, October 2, 1967.

2) The Influence of Machine Design on Numerical Algorithms, by W. J. Cody. Mathematics Department Colloquium, University of Missouri, Rolla, Missouri, November 21, 1967.

3) Generating Functions and Transport Theory: Relation to Diffusion Theory and Related Approximations, by I. K. Abu-Shumays. Battelle-Northwest, Richland, Washington, November 1967.

4) Generating Functions and Transport Theory: Basic Relations, by I. K. Abu-Shumays. University of Washington, Seattle, Washington, November 1967.

5) Mechanical Theorem-Proving by Resolution, by John Reynolds. Two guest lectures in course, Information Sciences 371, University of Chicago, December 5-7, 1967.

6) Automatic Computation of Data Set Definitions in LISP, by John C. Reynolds. University of California Colloquium, San Diego, California, January 25, 1968.

7) Research Results in Transport Theory, by I. K. Abu-Shumays. Iowa State University, Ames, Iowa, February 1968.

8) Error Bounds of One-Step Methods, by Franz Stetter. University of Missouri, Rolla, Missouri, March 5, 1968.

9) Automatic Computation of Data Set Definitions, by John Reynolds. Seminar, Computer Science Department, Stanford University, Stanford, California, March 13, 1968.

10) A Simple Typeless Language which Allows Complex Data Structure and Co-routines, by John Reynolds. Computer Science Department Seminar, Stanford University, Stanford, California, March 14, 1968.

11) Grammatical Covering, by John C. Reynolds. Computer Science Department Seminar, Stanford University, Stanford, California, March 19, 1968.

12) A Generalization of Resolution Using Context-Free Grammars, by John C. Reynolds. Computer Science Department Seminar, Stanford University, Stanford, California, March 21, 1968.

13) Inversion of Toeplitz Matrices, by Erwin Bareiss. Battelle-Northwest, Richland, Washington, April 25, 1968.

14) Spectral Theory of the Neutron Boltzman Equation, by Erwin Bareiss. Televised Seminar, Seattle, Washington, April 26, 1968.

15) Algorithmic Proof Procedures, by John C. Reynolds. Information Sciences 379, University of Chicago, Spring Quarter 1968.

16) Theorem Proving on the Computer, by Lawrence Wos. Mathematics Department Colloquium, Washington University, St. Louis, Missouri, May 17, 1968.

SEMINARS AND SYMPOSIA

Applied Mathematics Division Seminars

July 6, 1967	The Mathematical Interpretation of the Notion of Morphogenetic Field, by Professor R. Thom, Institut des Hautes Etudes Scientifique, Paris, and Visiting Professor, Brandeis University, Waltham, Massachusetts.
July 10, 1967	The Plasma Display - A New Technique for Information Storage and Display, by Dr. Gene Slottow, Coordinated Science Laboratory, University of Illinois, Urbana, Illinois.
July 13, 1967	Accurate Solution of Linear Algebraic Systems - A Survey, by Dr. Cleve B. Moler, Mathematics Department, The University of Michigan, Ann Arbor, Michigan.
July 20, 1967	Computer Generated Microfilm and 16 mm Movies, by Captain Neal Morgan, USAF, Air Force Weapons Laboratory, Kirtland Air Force Base, New Mexico.
July 27, 1967	Decision Procedures for Subcases of the Predicate Calculus, by Dr. Joyce Friedman, Computer Science Department, Stanford University, Stanford, California.
August 3, 1967	Error Bounds for Quadratures, by Dr. Frank Stenger, Department of Mathematics, The University of Michigan, Ann Arbor, Michigan.
August 17, 1967	DATATRAN: The Input Language for the Nova Modular Program System. Basic Philosophy and Experience, by Dr. H. J. Kopp, Knolls Atomic Power Laboratory, Schenectady, New York.
August 24, 1967	Construction of Gaussian Quadrature Formulas, by Professor Walter Gautschi, Division of Mathematical Sciences, Purdue University, Lafayette, Indiana.
August 31, 1967	C*-Algebras and Statistical Mechanics, by Dr. J.C.T. Pool, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
September 14, 1967	Numerical Algorithms Based on the Theory of Complex Variables, by Dr. James Lyness, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
September 28, 1967	A Generalization of Chandrasekhar's H-equation, by Dr. M. K. Nestell, Mathematics Department, Battelle Northwest, Richland, Washington.
October 11, 1967	The Spherically Symmetric Problems in Neutron Transport Theory, by Professor Roman Zelazny, Head of the Department of Mathematics, Institute of Nuclear Research, Swierk and Warsaw University, Poland.

October 19, 1967	Conversational Computing in PL/I, by Dr. R. L. Wexelblat, Bell Telephone Laboratories, Holmdel, New Jersey.
October 26, 1967	On Numerical Integration of the Differential Equations of Oscillating Phenomena, by Professor E. Stiefel, Swiss Institute of Technology, Zurich, Switzerland, and Yale University, Department of Astronomy, New Haven, Connecticut.
November 2, 1967	Psychedelic Physics or An Application of Computer Animation, by Dr. Ronald Blum, Department of Physics, The University of Chicago, Chicago, Illinois.
November 9, 1967	Character Strings in General Purpose Procedural Languages, by Professor Robert F. Rosin, Computer Center, Yale University, New Haven, Connecticut.
November 30, 1967	Ergodic Theory and Information, by Professor Patrick Billingsley, Department of Statistics, The University of Chicago, Chicago, Illinois.
December 13, 1967	A Survey of Error Analysis, by Professor William Kahan, Mathematics Department, University of Toronto, Toronto, Ont., Canada.
December 14, 1967	Can Photons be Localized? by Dr. J. M. Jauch, Director Institut de Physique Théorique, Université de Genève, Genève, Switzerland.
December 21, 1967	On the Analytic Continuation of the Resolvent Kernel in Scattering Theory, by Professor Calvin H. Wilcox, Department of Mathematics, The University of Arizona, Tucson, Arizona.
December 27, 1967	Some 1-Dimensional Models which Exhibit Phase Transitions, by Professor Mark Kac, Department of Mathematics, The Rockefeller University, New York, New York.
January 2, 1968	A Communication Based System 360, Model 75, by Professor Frederick P. Brooks, Jr., Chairman, Department of Information Science, The University of North Carolina, Chapel Hill, North Carolina.
January 4, 1968	Automatic Computation of Data Set Definitions in LISP, by Dr. John Reynolds, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
January 11, 1968	Potential Theory on Hilbert Space, by Professor L. Gross, Department of Mathematics, Massachusetts Institute of Technology, Cambridge, Massachusetts.
January 25, 1968	Dynamic Information Retrieval and Electron-Atom Collisions, by Professor Kenneth Smith, Institute of Computational Sciences, The University of Nebraska, Lincoln, Nebraska.

February 7, 1968	Marginal Cases in Potential Scattering Theory, by Dr. William M. Frank, U.S. Naval Ordnance Laboratory, Washington, D.C.
February 22, 1968	The Mathematical Structure of Empirical Logic, by Professor Charles H. Randall, Department of Mathematics, University of Massachusetts, Amherst, Massachusetts.
February 29, 1968	Convergent Perturbation Expansions for Quantum Field Theory, by Professor Reese T. Prosser, Department of Mathematics, Dartmouth College, Hanover, New Hampshire.
March 14, 1968	Symmetries of Algebras of Observables, by Professor R. V. Kadison, Department of Mathematics, University of Pennsylvania, Philadelphia, Pennsylvania.
March 21, 1968	Why Formal Definition? by Mr. T. B. Steel, Jr., Applied Technology Division, System Development Corporation, Santa Monica, California.
March 28, 1968	Holomorphic Functions with Prescribed Asymptotic Expansions, by Dr. F. Pittnauer, Department of Mathematics, University of Wisconsin, Madison, Wisconsin.
April 9, 1968	Congruential Random Number Generators Are No Good, by Dr. George Marsaglia, Boeing Scientific Research Laboratories, Seattle, Washington.
April 11, 1968	Optimization of Algebraic Translators, by Professor R. M. McClure, Computer Science Center, Southern Methodist University, Dallas, Texas.
April 18, 1968	A Survey of Symbol Manipulation Languages, by Mr. David J. Farber, Computer Sciences Department, The Rand Corporation, Santa Monica, California.
April 25, 1968	Random Integral Equations, by Professor A. T. Bharucha-Reid, Department of Mathematics, Wayne State University, Detroit, Michigan.
May 2, 1968	Existence and Construction of Solutions of Partial Differential Equations, by Professor Richard Courant, Courant Institute of Mathematical Sciences, New York University, New York, N.Y.
May 9, 1968	Bounds for the Eigenvalues of Non-negative Matrices, by Professor Josef Stoer, Department of Mathematics, University of California, San Diego - LaJolla, California.
May 10, 1968	Asymptotic Expansions for Discretized Eigenvalue Problems, by Professor R. Bulirsch, Department of Mathematics, University of California, San Diego - LaJolla, California.

May 16, 1968	Bounds for the Error of Linear Systems Using the Theory of Moments, by Professor G. H. Golub, Computer Science Department, Stanford University, Stanford, California.
May 23, 1968	Current Status of Quantum Field Theory Models, by Professor Arthur Jaffe, Department of Physics, Harvard University, Cambridge, Massachusetts.
May 28, 1968	Computation of Topological Models for Four Dimensional Fundamental Domains, by Professor Harvey Cohn, Department of Mathematics, University of Arizona, Tucson, Arizona.
June 4, 1968	Implementation of A Plex Processing System with Implicit Links, by Mr. Wilfred J. Hansen, Computer Science Department, Stanford University, Stanford, California.
June 11, 1968	Graph Program Models for Parallel Computation, by Professor W. F. Miller, Stanford Linear Accelerator Center, Stanford University, Stanford, California.
June 14, 1968	Global Convergence of QR Algorithm, by Dr. J. H. Wilkinson, Mathematics Division, National Physical Laboratory, Teddington, Middlesex, England.
June 17, 1968	Orthogonality Relations for Neutron Transport in Plane Geometry, by Professor Norman J. McCormick, Nuclear Engineering Department, University of Washington, Seattle, Washington.
June 20, 1968	On the Condition of a Matrix Arising in the Numerical Inversion of the Laplace Transform, by Professor Walter Gautschi, Division of Mathematical Sciences, Purdue University, Lafayette, Indiana.
June 27, 1968	A Recursive Relation for the Characteristic Polynomial of a Pentadiagonal Matrix, by Dr. Roland A. Sweet, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.

Applied Mathematics Division Special Interest Seminars

July 12, 1967	Control Data Digigraphic Systems, by Mr. Barrie Irish and Mr. H. P. Peterson, Control Data Digigraphic Laboratories, Burlington, Massachusetts.
October 6, 1967	The Bit Series 480 Systems, by Mr. John Bragg, Business Information Technology, Inc., Natick, Massachusetts.
November 7, 1967	Demonstration of several pieces of equipment by California Computer Products, Inc.
November 10, 1967	POLLY, by Mr. Donald Hodges, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
November 10, 1967	A Computer-Controlled Electron Microscope, by Mr. J. Butler, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
April 4, 1968	Demonstration of the SPATIAL DATA Model 501-1 3-D Plotter, by Mr. John Wyman, Spatial Data Systems, Goleta, California.

Transport Theory and Stochastic Processes

A seminar lecture series started on March 23, 1966 is continuing, with Dr. J. E. Moyal in charge. Seminars given by Dr. Peter J. Brockwell, Applied Mathematics Division; Dr. Ibrahim K. Abu-Shumays, Applied Mathematics Division.

Seminar on Mathematical Physics

This series was reactivated to provide a forum for the discussion of mathematical subjects related to the foundations of classical and quantum physics. Scheduled subjects include the lattice-theoretic approach to quantum mechanics, and topics from the theory of Lie groups and differential geometry. Dr. J. C. T. Pool in charge. Seminars given by: Dr. J. C. T. Pool, Applied Mathematics Division; Dr. J. M. Cook, Applied Mathematics Division; Dr. E. Thieleker, Applied Mathematics Division; Professor J. Chaiken, Department of Mathematics, Massachusetts Institute of Technology, Cambridge, Massachusetts; Professor John Dollard, Department of Mathematics, University of Rochester, Rochester, New York; Professor N. Shenk, Department of Mathematics, Columbia University, New York, N.Y.; Professor W. Faris, Department of Mathematics, Cornell University, Ithaca, New York; Professor G. W. Mackey, Department of Mathematics, Harvard University, Cambridge, Massachusetts.

Fluid Dynamics Conference

An informal conference entitled "Computational Methods in Fluid Dynamics" was held in the Applied Mathematics Division the first week in September, 1967. The purpose of the meeting was to provide an opportunity for intensive discussion of recent progress and current problems in the area of numerical fluid dynamics. Members of the Applied Mathematics Division were fortunate to be able to sit in on a number of informal talks by participants on their work. Active non-Argonne participants in the conference were: G. Birkhoff (Harvard University); B. J. Daly (Los Alamos); J. Deardorff (University of Washington); S. C. R. Dennis (University of Western Ontario); J. Douglas, Jr. (University of Chicago); J. Fromm (IBM); J. D. Hellums (Rice University); C. W. Hirt (Los Alamos); P. D. Lax (Courant Institute); D. K. Lilly (National Center for Atmospheric Research); K. Meyer (Los Alamos); P. Michael (Brookhaven); B. Noble (University of Wisconsin); W. F. Noh (Lawrence Radiation Laboratory - Livermore); C. E. Pearson (Boeing); J. P. Shannon (Los Alamos); R. S. Varga (Case Western Reserve University); C. Wilcox (University of Arizona) - (Organizer of the Conference); D. M. Young (University of Texas).